Access DB# _____

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: LEE, RICHARD A. Examiner # : 78680 Date: JULY 6, 2004
Art Unit: 1713 Phone Number ~~30~~ 571-272-1104 Serial Number: 10/624,679
Mail Box and Bldg/Room Location: REM10A21 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

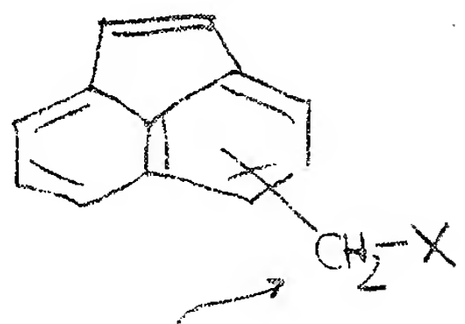
Title of Invention: ACENAPHTHYLENE DERIVATIVE, POLYMER, and ANTI-REFLECTIVE COMPOSITION

Inventors (please provide full names): SUGITA, H. KONNO, K.
TANAKA, M. SHIMOKAWA, T.

Earliest Priority Filing Date: July 31, 2002

***For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.**

Please search for acenaphthalene derivatives having the following general formula



must have methylene group
X can be anything

substituent CH_2X located on either six membered ring

STIC Search Report
EIC 1700

STIC Database Tracking Number: 126545

TO: Rip A Lee
Location: REM 10A24
Art Unit : 1713
July 12, 2004

Case Serial Number: 10/624670

From: Kathleen Fuller
Location: EIC 1700
REMSEN 4B28
Phone: 571/272-2505
Kathleen.Fuller@uspto.gov

Search Notes

Search and Information Resources Administration

STIC Search Results Feedback Form

EIC17000

Questions about the scope or the results of the search? Contact *the EIC searcher or contact*:

Kathleen Fuller, EIC 1700 Team Leader
571/272-2505 REMSEN 4B28

Voluntary Results Feedback Form

- *I am an examiner in Workgroup:* ☐ *Example: 1713*
- *Relevant prior art* ***found****, search results used as follows:*
  - ☐ 102 rejection
  - ☐ 103 rejection
  - ☐ Cited as being of interest.
  - ☐ Helped examiner better understand the invention.
  - ☐ Helped examiner better understand the state of the art in their technology.

Types of relevant prior art found:

- ☐ Foreign Patent(s)
- ☐ Non-Patent Literature
  (journal articles, conference proceedings, new product announcements etc.)

- *Relevant prior art* ***not found:***
  - ☐ Results verified the lack of relevant prior art (helped determine patentability).
  - ☐ Results were not useful in determining patentability or understanding the invention.

Comments:

Drop off or send completed forms to EIC1700 REMSEN 4B28

Access DB# _____

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: LEE, RICK A. Examiner #: 78680 Date: JULY 6, 2004
Art Unit: 1713 Phone Number ~~30~~ 571-272-1104 Serial Number: 10/624,679
Mail Box and Bldg/Room Location: ~~REM~~ 10A24 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

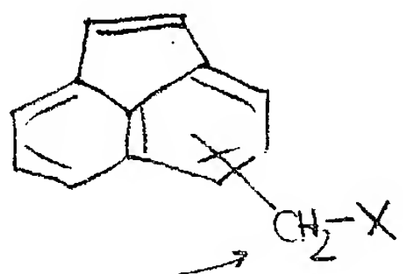
Title of Invention: ACENAPHTHYLENE DERIVATIVE, POLYMER, and ANTI-REFLECTIVE COMPOSITION

Inventors (please provide full names): SUGITA, H. KONNO, K.
TANAKA, M. SHIMOKAWA, T.

Earliest Priority Filing Date: July 31, 2002

***For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.**

Please search for acenephthalene derivatives having the following general formula



must have methylene group
X can be anything

substituent CH_2X located on either six membered ring

****

STAFF USE ONLY

Searcher: _____
Searcher Phone #: _____
Searcher Location: _____
Date Searcher Picked Up: _____
Date Completed: _____
Searcher Prep & Review Time: 20
Clerical Prep Time: _____
Online Time: 20

Type of Search

NA Sequence (#)_____
AA Sequence (#)_____
Structure (#) _____
Bibliographic _____
Litigation _____
Fulltext _____
Patent Family _____
Other _____

Vendors and cost where applicable

STN _____
Dialog _____
Questel/Orbit _____
Dr.Link _____
Lexis/Nexis _____
Sequence Systems _____
WWW/Internet _____
Other (specify) _____

PTO-1590 (8-01)

=> FILE REG
FILE 'REGISTRY' ENTERED AT 11:19:31 ON 12 JUL 2004

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 JUL 2004 HIGHEST RN 708207-86-7
DICTIONARY FILE UPDATES: 11 JUL 2004 HIGHEST RN 708207-86-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

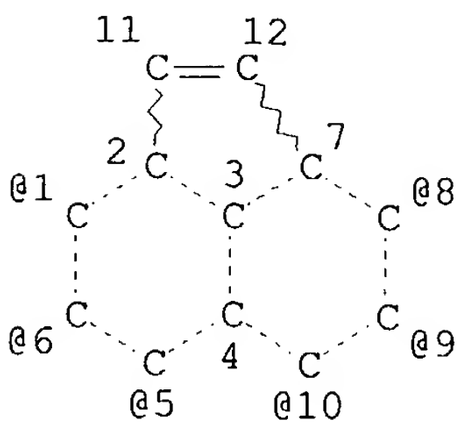
=> FILE HCAPLUS
FILE 'HCAPLUS' ENTERED AT 11:19:36 ON 12 JUL 2004

FILE COVERS 1907 - 12 Jul 2004 VOL 141 ISS 3
FILE LAST UPDATED: 11 Jul 2004 (20040711/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> D QUE L53
L50 STR

KATHLEEN FULLER EIC 1700 REMSEN 4B28 571/272-2505



76 structures from this query

CH2 @13

VPA 13-8/9/10/5/6/1 U
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE
L52 76 SEA FILE=REGISTRY SSS FUL L50
L53 39 SEA FILE=HCAPLUS ABB=ON L52

39 CA references

=> D L53 BIB ABS HITIND HITSTR 1-39

L53 ANSWER 1 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2004:97225 HCAPLUS
DN 140:136438
TI Acenaphthylene derivative, polymer, and antireflection film-forming composition
IN Sugita, Hikaru; Konno, Keiji; Tanaka, Masato; Shimokawa, Tsutomu
PA JSR Corporation, Japan
SO Eur. Pat. Appl., 26 pp.
CODEN: EPXXDW
DT Patent
LA English

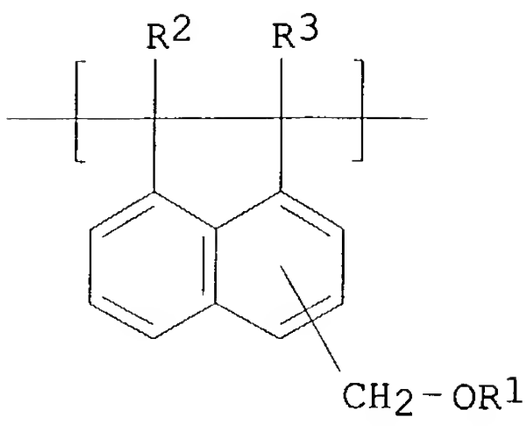
applicants

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1386904	A1	20040204	EP 2003-17282	20030730
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	US 2004034155	A1	20040219	US 2003-624678	20030723
	JP 2004168748	A2	20040617	JP 2003-283561	20030731
PRAI	JP 2002-224138	A	20020731		
	JP 2002-324709	A	20021108		

OS MARPAT 140:136438
GI

KATHLEEN FULLER EIC 1700 REMSEN 4B28 571/272-2505



I

AB Novel compds. acetoxymethylacenaphthylene and hydroxymethylacenaphthyleneare are disclosed. A polymer prepared from these novel compds. contains a structural unit of the formula I (R1 = H; R2,3 = monovalent atom or a monovalent organic group). The polymer is suitable as a component for an antireflection film-forming composition exhibiting a high antireflection effect and not causing intermixing with a resist film.

IC ICM C07C033-38
ICS C08F232-08; G03F007-09

CC 74-5 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 76

IT 510754-50-4P 650624-82-1P **650624-84-3P** 650624-86-5P
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(acenaphthylene derivative and polymer for antireflection film-forming composition)

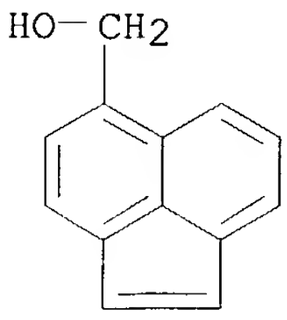
IT **650624-84-3P**
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(acenaphthylene derivative and polymer for antireflection film-forming composition)

RN 650624-84-3 HCAPLUS

CN 5-Acenaphthylenemethanol, polymer with acenaphthylene (9CI) (CA INDEX NAME)

CM 1

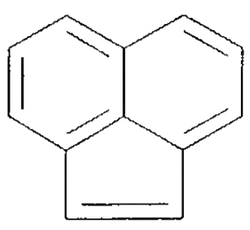
CRN 650624-83-2
CMF C13 H10 O



CM 2

KATHLEEN FULLER EIC 1700 REMSEN 4B28 571/272-2505

CRN 208-96-8
CMF C12 H8



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 2 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:834012 HCAPLUS
DN 138:60408
TI Investigation of the Volatile Organic Substances that Cause the Characteristic Odor of Pentachlorophenol Treated Wood Utility Poles
AU Fortin, Myriam; Gilbert, Roland; Besner, Andre; Labrecque, Jean-Francois; Hubert, Joseph
CS Institut de Recherche d'Hydro-Quebec, Varennes, QC, J3X 1S1, Can.
SO Environmental Science and Technology (2002), 36(23), 5014-5020
CODEN: ESTHAG; ISSN: 0013-936X
PB American Chemical Society
DT Journal
LA English
AB The nature of volatile organic compds. which could be the origin of the characteristic odor of treated wood utility poles was studied by examining compositional changes in the chromatog. profiles of fresh pentachlorophenol (PCP) solvent samples and weathered samples collected from an in-service red pine pole. More than 99 peaks were identified in the fresh solvent chromatogram from which a large portion of the C3-, C4-, C5-, C6-alkylbenzene isomers and early eluting n-alkanes was missing from the anal. of weathered samples. Three domains in the chromatog. profile (volatile, semi-volatile, non-volatile components) were confirmed by assessing the headspace of fresh PCP solvent samples using direct syringe sampling and solid-phase micro-extraction A first level of field validation was achieved using an emission cell to measure substances emanating from sapwood specimens at different temps. Average latent heat of vaporization (ΔHvap) of PCP solvent components was estimated to be 99.9 kJ/mol from these results. Anal. of airborne substances at a treating plant and utility pole storage site confirmed the C4-, C5-, and C6-alkylbenzene isomers could contribute to the characteristic odor perceived by humans.
CC 59-2 (Air Pollution and Industrial Hygiene)
Section cross-reference(s): 43, 80
IT 71-43-2, Benzene, analysis 83-32-9, Acenaphthene 85-01-8, Phenanthrene, analysis 86-73-7, Fluorene 90-12-0, 1-Methylnaphthalene 91-20-3, Naphthalene, analysis 91-57-6, 2-Methylnaphthalene 92-52-4, Biphenyl, analysis 95-47-6, o-Xylene, analysis 95-63-6, 1,2,4-Trimethylbenzene 95-93-2, 1,2,4,5-Tetramethylbenzene 98-82-8, Isopropylbenzene 99-87-6, p-Cymene 100-41-4, Ethylbenzene, analysis 103-65-1, Propylbenzene 104-51-8, 1-Butylbenzene 105-05-5, 1,4-Diethylbenzene 106-42-3, p-Xylene, analysis 108-38-3, m-Xylene, analysis 108-67-8, 1,3,5-Trimethylbenzene, analysis 108-88-3, Toluene, analysis 112-40-3, Dodecane 112-95-8, Eicosane 119-64-2, 1,2,3,4-Tetrahydronaphthalene 120-12-7, Anthracene, analysis 124-18-5, Decane 135-01-3, 1,2-Diethylbenzene 135-98-8, sec-Butylbenzene

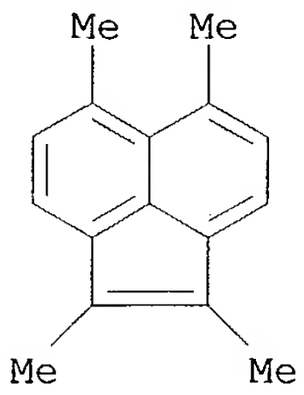
141-93-5, 1,3-Diethylbenzene 208-96-8, Acenaphthylene 275-51-4, Azulene 475-03-6, 1,2,3,4-Tetrahydro-1,1,6-trimethylnaphthalene 488-23-3, Benzene, 1,2,3,4-Tetramethyl- 490-65-3, Naphthalene, 1-Methyl-7-(1-methylethyl)- 496-11-7, 2,3-Dihydro-1H-indene 527-53-7, 1,2,3,5-Tetramethylbenzene 535-77-3, m-Cymene 538-68-1, Amylbenzene 544-76-3, Hexadecane 575-41-7, 1,3-Dimethylnaphthalene 581-40-8, 2,3-Dimethylnaphthalene 581-42-0, 2,6-Dimethylnaphthalene 593-45-3, Octadecane 611-14-3, 1-Ethyl-2-methylbenzene 613-33-2, 4,4'-Dimethylbiphenyl 620-14-4, 1-Ethyl-3-methylbenzene 629-50-5, Tridecane 629-59-4, Tetradecane 629-62-9, Pentadecane 629-78-7, Heptadecane 629-92-5, Nonadecane 629-94-7, Heneicosane 629-97-0, Docosane 629-99-2, Pentacosane 638-67-5, Tricosane 646-31-1, Tetracosane 767-58-8, 2,3-Dihydro-1-methyl-1H-indene 781-43-1, 9,10-Dimethylanthracene 832-69-9, 1-Methylphenanthrene 874-41-9, 1-Ethyl-2,4-dimethylbenzene 934-74-7, 1-Ethyl-3,5-dimethylbenzene 934-80-5, 4-Ethyl-1,2-dimethylbenzene 939-27-5, 2-Ethylnaphthalene 1074-17-5, 1-Methyl-2-propylbenzene 1074-43-7, 1-Methyl-3-propylbenzene 1074-55-1, 1-Methyl-4-propylbenzene 1075-22-5 1076-61-5, 1,2,3,4-Tetrahydro-6,7-dimethylnaphthalene 1077-16-3, Hexylbenzene 1120-21-4, Undecane 1127-76-0, 1-Ethylnaphthalene 1207-15-4 1430-97-3, 2-Methyl-9H-fluorene 1559-81-5, 1,2,3,4-Tetrahydro-1-methylnaphthalene 1576-67-6, 3,6-Dimethylphenanthrene 1595-16-0, Benzene, 1-Methyl-4-(1-methylpropyl)- 1758-85-6, Benzene, 2,4-Diethyl-1-methyl- 1758-88-9, 2-Ethyl-1,4-dimethylbenzene 1921-70-6, 2,6,10,14-Tetramethylpentadecane 2027-17-0, Naphthalene, 2-(1-Methylethyl)- 2245-38-7, 2,3,5-Trimethylnaphthalene 2809-64-5, 1,2,3,4-Tetrahydro-5-methylnaphthalene 3031-15-0, 1,2,3,4-Tetramethylnaphthalene 3674-66-6, 2,5-Dimethylphenanthrene 3877-19-8, 1,2,3,4-Tetrahydro-2-methylnaphthalene 4175-54-6, Naphthalene, 1,2,3,4-Tetrahydro-1,4-dimethyl- 4612-63-9, 2,3-Dimethyl-9H-fluorene 6682-71-9 13065-07-1, Naphthalene, 1,2,3,4-Tetrahydro-2,7-dimethyl- 16587-52-3, 3-Methyldibenzothiophene 17059-48-2 21164-95-4, 7,9-Dimethylhexadecane 21564-91-0, 1,2,3,4-Tetrahydro-1,5-dimethylnaphthalene 21693-54-9, 1,2,3,4-Tetrahydro-5,7-dimethylnaphthalene 21693-55-0, Naphthalene, 1,2,3,4-Tetrahydro-1,5,7-trimethyl- 25550-13-4, Diethylmethylbenzene 28652-77-9, Trimethylnaphthalene 30316-17-7, 1,2,3,4-Tetrahydro-2,5,8-trimethylnaphthalene 33930-85-7 40650-41-7 42775-75-7, 5-Ethyl-1,2,3,4-tetrahydronaphthalene 56147-63-8 **132118-73-1**, Acenaphthylene, 1,2,5,6-Tetramethyl-
RL: ANT (Analyte); OCU (Occurrence, unclassified); POL (Pollutant); ANST (Analytical study); OCCU (Occurrence)
(volatile organic compds. causing characteristic odor from pentachlorophenol-treated wood utility poles determined by measuring compositional changes in chromatog. profiles of fresh and weathered solvent samples)

IT **132118-73-1**, Acenaphthylene, 1,2,5,6-Tetramethyl-
RL: ANT (Analyte); OCU (Occurrence, unclassified); POL (Pollutant); ANST (Analytical study); OCCU (Occurrence)
(volatile organic compds. causing characteristic odor from pentachlorophenol-treated wood utility poles determined by measuring compositional changes in chromatog. profiles of fresh and weathered solvent samples)

RN 132118-73-1 HCAPLUS

CN Acenaphthylene, 1,2,5,6-tetramethyl- (9CI) (CA INDEX NAME)

KATHLEEN FULLER EIC 1700 REMSEN 4B28 571/272-2505



RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 3 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:547252 HCAPLUS
DN 137:109970
TI Acenaphthylene ring-containing crosslinkable compounds, their intermediates, their manufacture, and cured products
IN Honda, Hiroshi
PA Hitachi Chemical Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 2002205967	A2	20020723	JP 2001-3423	20010111
PRAI JP 2001-3423		20010111		

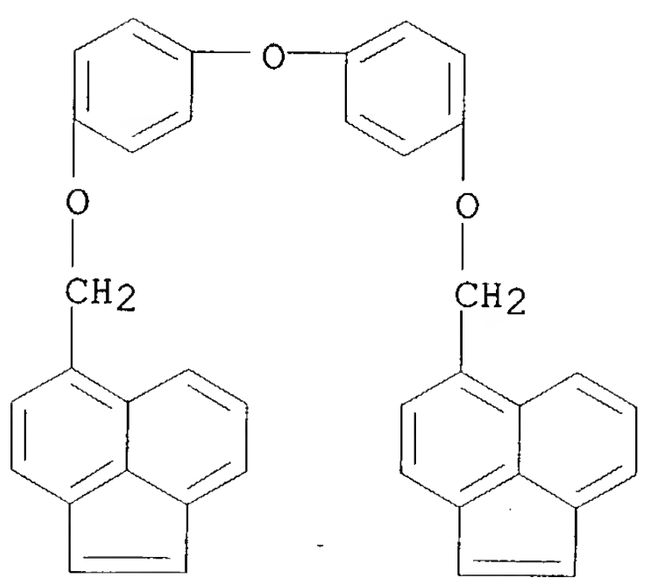
OS MARPAT 137:109970
AB Crosslinkable compds. (QCH2O)nR (I; Q = acenaphthylen-5-yl; n = pos. integer; R = n-valent organic group) and their intermediates QCH2X (II; Q = same as I; X = halo) are claimed. Thus, etherification of 4,4'-dihydroxydiphenyl ether with II (X = Cl) gave 55.8% I (n = 2, R = p-C6H4OC6H4-p), which gave a cured product at 151°.
IC ICM C07C043-285
ICS C07C017-357; C07C022-04; C07C041-16; C08F032-08; C08K005-06; C08L101-00
CC 37-2 (Plastics Manufacture and Processing)
Section cross-reference(s): 25
IT **443282-80-2P**
RL: IMF (Industrial manufacture); PREP (Preparation)
(manufacture of acenaphthylene ring-containing crosslinkable compds. and their intermediates)
IT 5345-46-0P, 5-Formylacenaphthene 50773-22-3P 62456-13-7P, 5-Chloromethylacenaphthene **443282-78-8P 443282-79-9P**
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(manufacture of acenaphthylene ring-containing crosslinkable compds. and their intermediates)
IT **443282-80-2P**
RL: IMF (Industrial manufacture); PREP (Preparation)
(manufacture of acenaphthylene ring-containing crosslinkable compds. and their intermediates)

KATHLEEN FULLER EIC 1700 REMSEN 4B28 571/272-2505

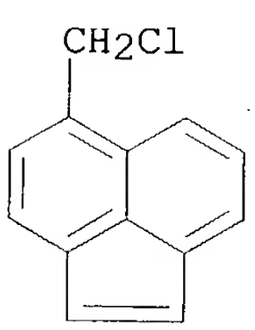
RN 443282-80-2 HCAPLUS
CN Acenaphthylene, 5,5'-[oxybis(4,1-phenyleneoxymethylene)]bis-, homopolymer (9CI) (CA INDEX NAME)

CM 1

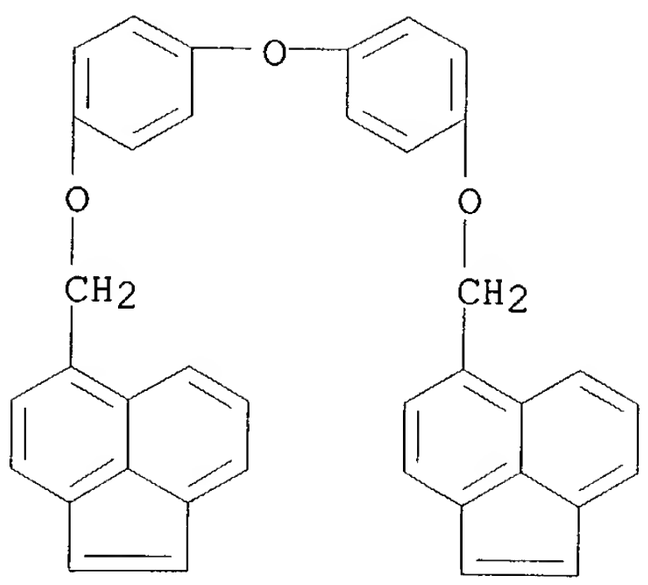
CRN 443282-79-9
CMF C38 H26 O3



IT **443282-78-8P 443282-79-9P**
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(manufacture of acenaphthylene ring-containing crosslinkable compds. and their
intermediates)
RN 443282-78-8 HCAPLUS
CN Acenaphthylene, 5-(chloromethyl)- (9CI) (CA INDEX NAME)

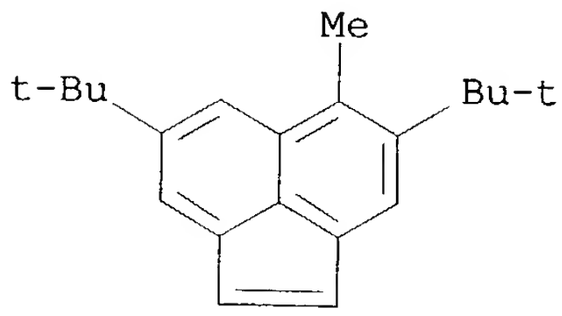


RN 443282-79-9 HCAPLUS
CN Acenaphthylene, 5,5'-[oxybis(4,1-phenyleneoxymethylene)]bis- (9CI) (CA INDEX NAME)



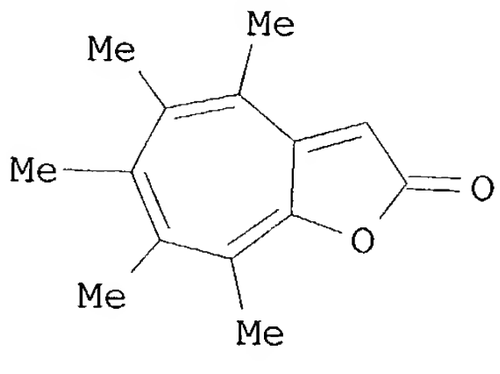
L53 ANSWER 4 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:779945 HCAPLUS
DN 136:232106
TI Tetra-tert-butyl-as-indaceno[1,2,3-cd:6,7,8-c'd']diphenalene: a four-stage amphoteric redox system
AU Kubo, Takashi; Yamamoto, Kagetoshi; Nakasuji, Kazuhiro; Takui, Takeji
CS Graduate School of Science, Department of Chemistry, Osaka University, Toyonaka, 560-0043, Japan
SO Tetrahedron Letters (2001), 42(45), 7997-8001
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 136:232106
AB Tetra-tert-butyl-as-indaceno[1,2,3-cd:6,7,8-c'd']diphenalene (TTB-as-IDPL) was prepared and found to behave as a four-stage amphoteric redox compound The properties of its five redox states were investigated. Properties of the newly synthesized compound were compared to the known, sym. 4,8,12,16-tetrakis(1,1-dimethylethyl)benz[5,6]acenaphtho[1,2-k]benzo[cd]fluoranthene.
CC 25-29 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 22
IT 105-53-3, Diethyl malonate 108-31-6, Maleic anhydride, reactions
203726-97-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of tetra-tert-butyl-as-indaceno[1,2,3-cd:6,7,8-c'd']diphenalene and its properties as four-stage amphoteric redox system)
IT **203726-97-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of tetra-tert-butyl-as-indaceno[1,2,3-cd:6,7,8-c'd']diphenalene and its properties as four-stage amphoteric redox system)
RN 203726-97-0 HCAPLUS
CN Acenaphthylene, 4,7-bis(1,1-dimethylethyl)-5-methyl- (9CI) (CA INDEX NAME)

KATHLEEN FULLER EIC 1700 REMSEN 4B28 571/272-2505



RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 5 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:561252 HCAPLUS
DN 135:318178
TI Surprising formation of highly substituted azulenes on thermolysis of 4,5,6,7,8-pentamethyl-2H-cyclohepta[b]furan-2-one and heptalene formation with the new azulenes
AU Lellek, Vit; Hansen, Hans-Jurgen
CS Organisch-chemisches Institut der Universitat Zurich, Zurich, CH-8057, Switz.
SO Helvetica Chimica Acta (2001), 84(6), 1712-1736
CODEN: HCACAV; ISSN: 0018-019X
PB Verlag Helvetica Chimica Acta
DT Journal
LA English
OS CASREACT 135:318178
GI



I

AB Heating of 4,5,6,7,8-pentamethyl-2H-cyclohepta[b]furan-2-one (1a, I) in decalin at temps. > 170° leads to the development of a blue color, typical for azulenes. It belongs, indeed, to two formed azulenes, namely 4,5,6,7,8-pentamethyl-2-(2,3,4,5,6-pentamethylphenyl)azulene (4a) and 4,5,6,7,8-pentamethylazulene (5a). As a third product, 4,5,6,7-tetramethyl-2-(2,3,4,5,6-pentamethylphenyl)-1H-indene (6a) is also found in the reaction mixture Neither 4,6,8-trimethyl-2H-cyclohepta[b]furan-2-one (1b) nor 2H-cyclohepta[b]furan-2-one (1c) exhibit, on heating, such reactivity. However, heating of mixts. 1a/1b or 1a/1c results in the formation of crossed azulenes, namely 4,6,8-trimethyl-2-(2,3,4,5,6-pentamethylphenyl)azulene (4ba) and 2-(2,3,4,5,6-pentamethylphenyl)azulene (4ca), resp. The formation of small amts. of 4,6,8-trimethylazulene (5ba) and azulene (5ca), resp., besides 1H-indene 6a is also observed The observed product types speak for an [8+2]-cycloaddn. reaction between two mols. of 1a or between 1b and 1c, resp., with 1a, whereby 1a plays in the latter two cases the part of the two-atom component. Strain release, due to the five adjacent Me groups in 1a, in the [8+2]-cycloaddn. step seems to be

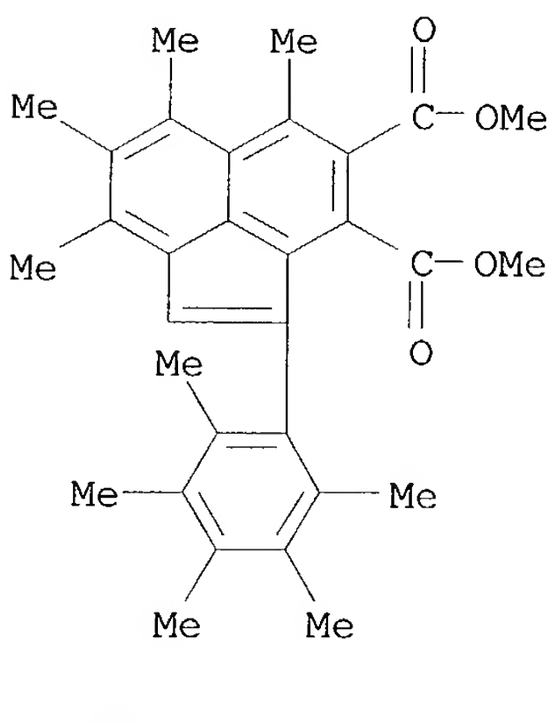
the driving force for these transformations, which are further promoted by the consecutive loss of two mols. of CO2 and concomitant formation of the 10π-electron system of the azulenes. The new azulenes react with di-Me acetylenedicarboxylate (ADM) to form the corresponding di-Me heptalene-4,5-dicarboxylates, which give thermally or photochem. the corresponding double-bond-shifted (DBS) isomers. The five adjacent Me groups in exert a certain buttressing effect, whereby their thermal DBS process is distinctly retarded in comparison to rings which carry "isolated" Me groups. This view is supported by X-ray crystal-structure analyses.

CC 22-5 (Physical Organic Chemistry)
Section cross-reference(s): 75

IT **367452-56-0P**
RL: BYP (Byproduct); PRP (Properties); PREP (Preparation)
(crystallog.; preparation of azulenes via chemoselective [2+8]-cycloaddn./cycloreversion/ring contraction from 2H-cyclohepta[b]furan-2-ones, and heptalene bond-shift isomers from the new azulenes + DMAD)

IT **367452-56-0P**
RL: BYP (Byproduct); PRP (Properties); PREP (Preparation)
(crystallog.; preparation of azulenes via chemoselective [2+8]-cycloaddn./cycloreversion/ring contraction from 2H-cyclohepta[b]furan-2-ones, and heptalene bond-shift isomers from the new azulenes + DMAD)

RN 367452-56-0 HCAPLUS
CN 3,4-Acenaphthylenedicarboxylic acid, 5,6,7,8-tetramethyl-2-(pentamethylphenyl)-, dimethyl ester (9CI) (CA INDEX NAME)



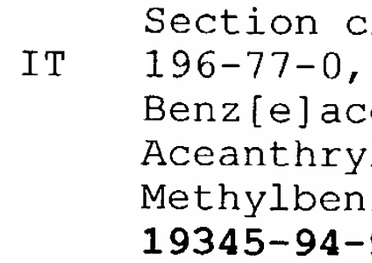
RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 6 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:231997 HCAPLUS
DN 130:303552
TI Classification of select aceanthrylenes, acephenanthrylenes, and dicyclopentapyrenes as alternant versus nonalternant polycyclic aromatic hydrocarbons on the basis of their fluorescence quenching behavior in the presence of nitromethane and cetylpyridinium cation selective quenching agents
AU Pandey, Siddharth; Acree, William E., Jr.; Scott, Lawrence T.; Necula, Atena; Fetzer, John C.; Mulder, Patrick P. J.; Lugtenburg, Johan;

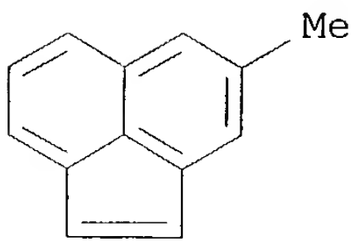
Cornelisse, Jan
CS Department Chemistry, University North Texas, Denton, TX, 76203, USA
SO Polycyclic Aromatic Compounds (1999), 13(1), 79-92
CODEN: PARCEO; ISSN: 1040-6638
PB Gordon & Breach Science Publishers
DT Journal
LA English
AB Fluorescence behavior of dicyclopenta[cd,fg]pyrene, dicyclopenta[cd,jk]pyrene and dicyclopenta[cd,mn]pyrene is reported in the presence of MeNO2 and cetylpyridinium (CPy+) cation quenching agents. MeNO2 and CPy+ are known to selectively quench fluorescence emission of alternant polycyclic aromatic hydrocarbons (PAHs). Emission intensities of nonalternant PAHs, with a few noted exceptions, are unaffected. Exptl. measurements show that MeNO2 and CPy+ effectively quenched fluorescence emission of the 3 dicyclopentapyrenes, thus suggesting that the perimeter C:C double bonds in the 2 cyclopenta-rings are alkenic, rather than aromatic in nature. Also reported are the fluorescence properties of 14 aceanthrylene and acephenanthrylene derivs., as well as several structurally related compds., to further document the cetylpyridinium cation's quenching selectivity.
CC 73-5 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): 22
IT 196-77-0, Benzo[def]cyclopenta[hi]chrysene 199-54-2, Benz[e]aceanthrylene 201-06-9, Acephenanthrylene 202-03-9, Aceanthrylene 208-96-8, Acenaphthylene 3343-10-0, 3-Methylbenz[j]aceanthrylene 7259-03-2 17057-80-6 18086-45-8 **19345-94-9**, 3-Methylacenaphthylene 19345-96-1 **19345-97-2**, 4-Methylacenaphthylene 19345-99-4, 1-Methylacenaphthylene 27208-37-3, Cyclopenta[cd]pyrene 39622-49-6 127229-46-3, Benz[j]aceanthrylene, 6-methyl-
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(fluorescence quenching of aceanthrylenes and acephenanthrylenes in cetylpyridinium chloride + cetyltrimethylammonium bromide micellar solns.)

IT **19345-94-9**, 3-Methylacenaphthylene **19345-97-2**, 4-Methylacenaphthylene
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(fluorescence quenching of aceanthrylenes and acephenanthrylenes in cetylpyridinium chloride + cetyltrimethylammonium bromide micellar solns.)

RN 19345-94-9 HCAPLUS
CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)

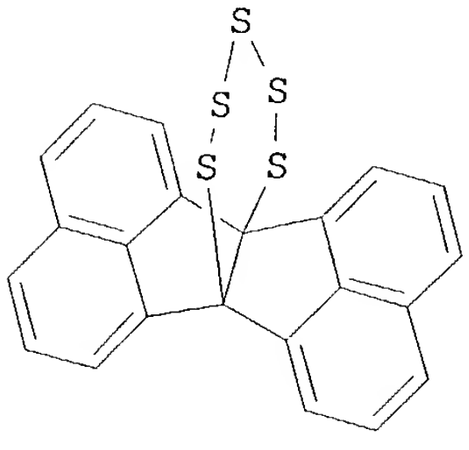


RN 19345-97-2 HCAPLUS
CN Acenaphthylene, 4-methyl- (8CI, 9CI) (CA INDEX NAME)



RE.CNT 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

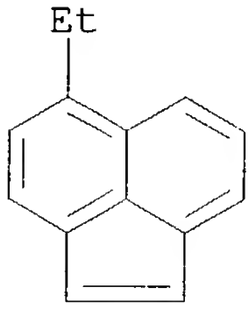
L53 ANSWER 7 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:197042 HCAPLUS
DN 130:311777
TI Synthesis of pentathiepanes and isolation of the conformers based on high inversion barrier of the pentathiepane ring
AU Sugihara, Yoshiaki; Takeda, Hitoshi; Nakayama, Juzo
CS Department Chemistry, Faculty Science, Saitama University, Urawa, 338, Japan
SO European Journal of Organic Chemistry (1999), (3), 597-605
CODEN: EJOCFK; ISSN: 1434-193X
PB Wiley-VCH Verlag GmbH
DT Journal
LA English
OS CASREACT 130:311777
GI



I

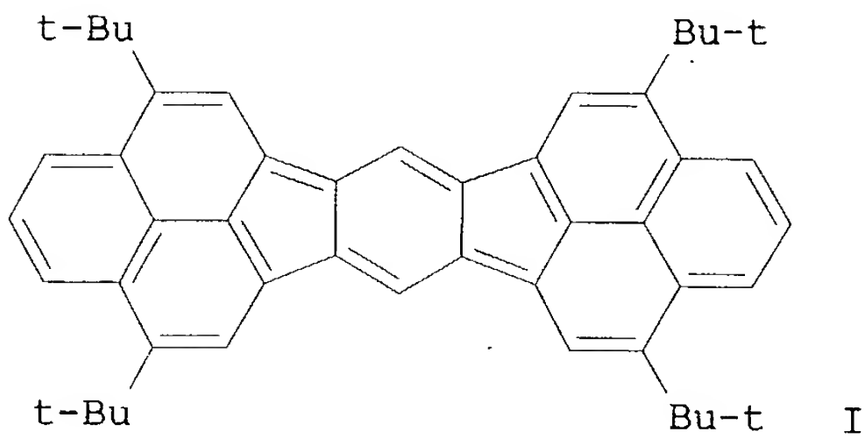
AB Acenaphtho[1,2-a]acenaphthylene was sulfurated with elemental S to give pentathiepane I. A dynamic NMR spectrum anal. revealed that the 2 naphthalene rings of I are chemical nonequivalent ≤100°. The pentathiepane ring of I adopts a chair conformation both in solution and crystals. In accordance with NMR, the sulfuration of 5-phenylacenaphtho[1,2-a]acenaphthylene gave a pair of conformers, which were isolated in pure form. The Friedel-Crafts acetylation of I, followed by dithioacetalization with HS(CH2)2SH, also gave a pair of isolable conformers. These 2 pairs of conformers isomerized, as a result of the ring inversion, to each other in solution at room temperature in the 1st-order kinetics. The activation parameters for this process, Ea, ΔH.thermod., and ΔS.thermod., were determined Based on the exptl. observations, a probable mechanism for the inversion process is proposed.
CC 28-22 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 22, 75

IT 10047-18-4P, 5-Acetylacenaphthene 13936-05-5P, 5-Ethylacenaphthene
56252-14-3P 110864-35-2P 207606-15-3P 223518-14-7P
223518-16-9P 223518-23-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and conformation of pentathiepanes)
IT **223518-16-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and conformation of pentathiepanes)
RN 223518-16-9 HCAPLUS
CN Acenaphthylene, 5-ethyl- (9CI) (CA INDEX NAME)



RE.CNT 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 8 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:150208 HCAPLUS
DN 128:204534
TI 4,8,12,16-Tetra-tert-butyl-s-indaceno[1,2,3-cd:5,6,7-c'd']diphenalene: a four-stage amphoteric redox system
AU Ohashi, Kenji; Kubo, Takashi; Masui, Takashi; Yamamoto, Kagetoshi; Nakasuji, Kazuhiro; Takui, Takeji; Kai, Yasushi; Murata, Ichiro
CS Department of Chemistry Graduate School of Science, Osaka University, Toyonaka, 560, Japan
SO Journal of the American Chemical Society (1998), 120(9), 2018-2027
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
OS CASREACT 128:204534
GI



I

AB A 4-stage amphoteric redox hydrocarbon (I) containing 2 phenalenyl units was prepared X-ray crystallog. of I reveals a delocalized D2h structure, which

is consistent with the presence of only 5 signals in the 1H NMR spectrum of I at -60°. The cyclic voltammogram of I exhibits 4 reversible redox waves with a small numerical sum (E1sum) of 1st oxidation (E1ox) and reduction (E1red) potentials. Four redox states of I were successfully generated from the neutral I, and were characterized by NMR, ESR and UV-visible-near-IR spectroscopies and theor. calcns. These spectral data reveal that phenalenyl units play an important role in the high amphotericity of I and the stability of the redox states generated.

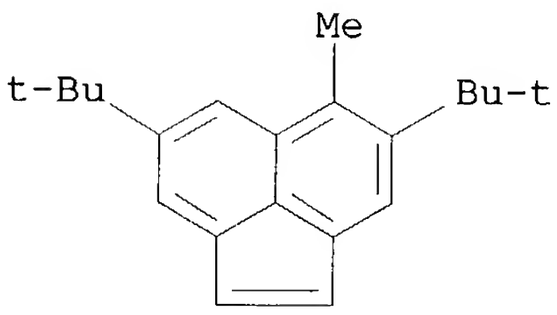
CC 22-7 (Physical Organic Chemistry)

IT **203726-97-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(tetra-tert-butylindacenodiphenalene synthesis as four-stage amphoteric redox system)

IT **203726-97-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(tetra-tert-butylindacenodiphenalene synthesis as four-stage amphoteric redox system)

RN 203726-97-0 HCAPLUS

CN Acenaphthylene, 4,7-bis(1,1-dimethylethyl)-5-methyl- (9CI) (CA INDEX NAME)



RE.CNT 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 9 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1997:126870 HCAPLUS

DN 126:238774

TI A new method for chemical modification of conductive polypyrroles without destroying their conductivity

AU Ono, Noboru; Tsukamura, Chikanori; Nomura, Youta; Hironaga, Hideo; Murashima, Takashi; Ogawa, Takuji

CS Faculty Science, Ehime University, Matsuyama, 790, Japan

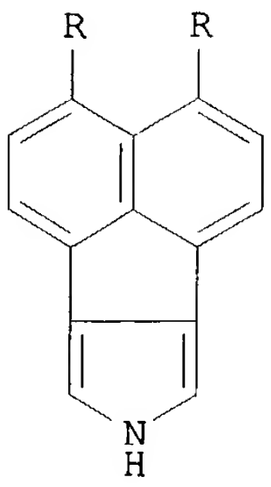
SO Advanced Materials (Weinheim, Germany) (1997), 9(2), 149-153
CODEN: ADVMEW; ISSN: 0935-9648

PB VCH

DT Journal

LA English

GI



I

AB The electropolymn. of I (R = H, Cl, Me, n-C6H13) gave modified polypyrroles with electronic and phys. properties that could be controlled by varying R. The polymers have extended π-conjugation and good conductivity, which was not reduced by the introduction of substituents in the fused aromatic rings. I polymers showed a reversible and stable electrochromism, and were very stable in both the doped and undoped state. Also UV/VIS and fluorescence spectra of the polymers were measured.

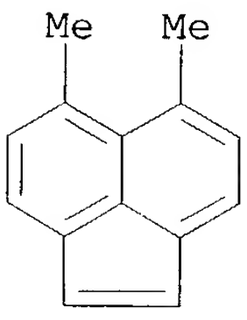
CC 35-7 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 36, 72, 73

IT 208-96-8, Acenaphthylene 7267-09-6 **41002-83-9**
188240-45-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(in preparation of pyrrole derivs. for electropolymn. to modified polypyrroles with retention of conductivity)

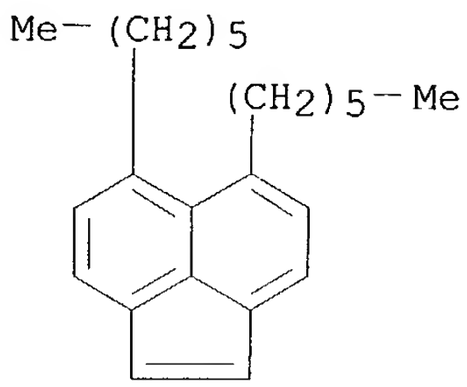
IT 13132-28-0P, 1-Nitroacenaphthylene 144991-40-2P **188240-44-0P**
188240-46-2P **188240-47-3P** 188240-48-4P 188240-49-5P
188240-50-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(in preparation of pyrrole derivs. for electropolymn. to modified polypyrroles with retention of conductivity)

IT **41002-83-9 188240-45-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(in preparation of pyrrole derivs. for electropolymn. to modified polypyrroles with retention of conductivity)

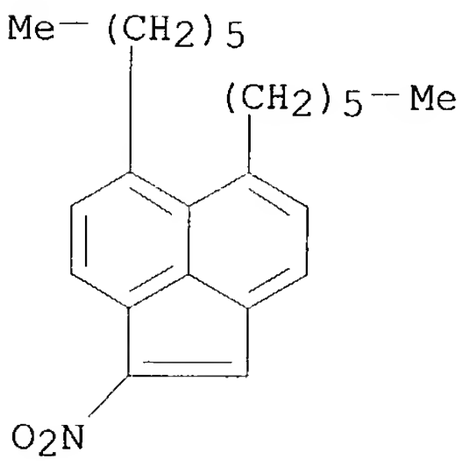
RN 41002-83-9 HCAPLUS
CN Acenaphthylene, 5,6-dimethyl- (6CI, 9CI) (CA INDEX NAME)



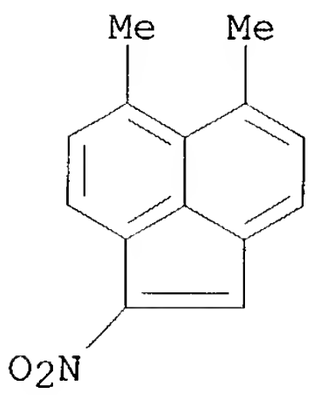
RN 188240-45-1 HCAPLUS
CN Acenaphthylene, 5,6-dihexyl- (9CI) (CA INDEX NAME)



IT **188240-44-0P 188240-47-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(in preparation of pyrrole derivs. for electropolymn. to modified polypyrroles with retention of conductivity)
RN 188240-44-0 HCAPLUS
CN Acenaphthylene, 5,6-dihexyl-1-nitro- (9CI) (CA INDEX NAME)



RN 188240-47-3 HCAPLUS
CN Acenaphthylene, 5,6-dimethyl-1-nitro- (9CI) (CA INDEX NAME)



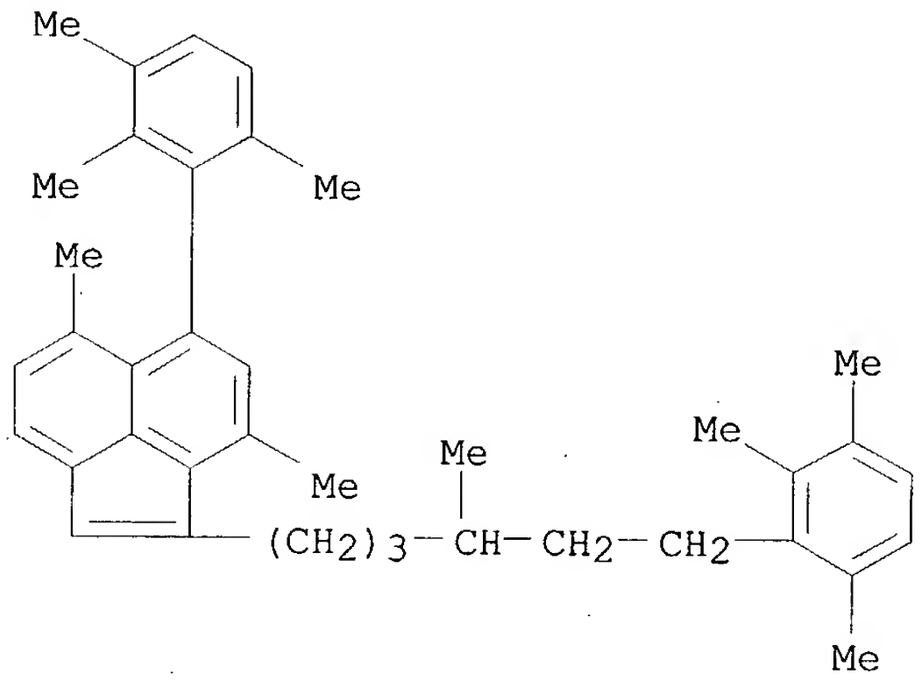
L53 ANSWER 10 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:46295 HCAPLUS
DN 126:173886
TI Diagenetic and catagenetic products of isorenieratene: molecular indicators for photic zone anoxia
AU Koopmans, Martin P.; Koster, Juergen; van Kaam-Peters, Heidy M. E.; Kenig, Fabien; Schouten, Stefan; Hartgers, Walter A.; de Leeuw, Jan W.; Damste, Jaap S. Sinninghe
CS Dep. Marine Biogeochem. Toxicol., Netherlands Inst. Sea Res. (NIOZ), Den

Burg, 1790 AB, Neth.
SO Geochimica et Cosmochimica Acta (1996), 60(22), 4467-4496
CODEN: GCACAK; ISSN: 0016-7037
PB Elsevier
DT Journal
LA English
AB A wide range of novel diagenetic and catagenetic products of the diarom. carotenoid isorenieratene, a pigment of the photosynthetic green sulfur bacteria Chlorobiaceae, were identified in a number of sedimentary rocks ranging from Ordovician to Miocene. Atropisomers contain an axially chiral center which, in combination with other chiral centers, resulted in two or more diastereomers that can be separated on a normal GC column. Because Chlorobiaceae-derived biomass is enriched in 13C, high 13C contents of isorenieratene derivs. support their inferred origins. These derivs. include C40-, C33-, and C32-diaryl isoprenoids and short-chain aryl isoprenoids with addnl. aromatic and/or S-containing rings. C33 and C32 compds. are diagenetic products of C33 and C32 "carotenoids" formed from isorenieratene during early diagenesis through expulsion of toluene and m-xylene, resp. Cyclization of the polyene acyclic isoprenoid chain can proceed via an intramol. Diels-Alder reaction, followed by aromatization of the newly formed ring. Sulphurization is also an important process during early diagenesis, competing with expulsion and cyclization. The inherent presence of a conjugated double bond system in carotenoids implies that similar diagenetic and catagenetic reactions can occur with all carotenoids. Because Chlorobiaceae live at or below the oxic/anoxic boundary layer and require both light and H2S, the presence of isorenieratene or its diagenetic and catagenetic products in ancient sedimentary rocks and crude petroleums is an excellent indication for photic zone anoxia in the depositional environment. Thus, these diagenetic and catagenetic products of isorenieratene can be used in reconstruction of palaeoenvironments and in oil-oil and oil-source rock correlation studies. Their presence in several petroleum source rocks suggested that anoxia is an important environmental parameter for the preservation of organic matter.
CC 51-1 (Fossil Fuels, Derivatives, and Related Products)
Section cross-reference(s): 53, 61
IT 153402-53-0 161269-47-2 187162-36-3 187162-38-5 187162-40-9
187162-42-1 187162-44-3 187162-46-5 187162-48-7 187162-50-1
187162-52-3 187162-54-5 187162-56-7 187162-58-9 **187162-60-3**
187162-62-5 187162-64-7 187162-66-9 187162-68-1 187162-70-5
187162-72-7 187162-74-9 187162-76-1 187162-78-3 187162-80-7
187162-83-0 187162-85-2 187162-87-4 187162-90-9 187162-92-1
187162-94-3 187162-96-5 187162-98-7 187163-00-4 187163-02-6
187163-04-8 187163-06-0 187163-08-2 187163-10-6 187163-12-8
187163-14-0 187163-16-2 187163-18-4 187163-20-8 187163-22-0
187163-24-2 187163-26-4 187163-28-6 187163-30-0 187163-32-2
187163-34-4 187163-36-6 187163-38-8 187163-39-9 187163-41-3
187163-44-6 187163-46-8 187163-48-0 187163-50-4 187163-52-6
187163-54-8 187163-56-0 187163-58-2 187163-60-6 187163-62-8
187163-64-0 187163-65-1 187163-66-2 187163-67-3 187163-68-4
187163-69-5 187163-70-8
RL: GFM (Geological or astronomical formation); GOC (Geological or astronomical occurrence); GPR (Geological or astronomical process); FORM (Formation, nonpreparative); OCCU (Occurrence); PROC (Process)
(diagenetic and catagenetic products of isorenieratenes as biomarkers for photic zone anoxia in petroleum genesis)
IT **187162-60-3**
RL: GFM (Geological or astronomical formation); GOC (Geological or astronomical occurrence); GPR (Geological or astronomical process); FORM

(Formation, nonpreparative); OCCU (Occurrence); PROC (Process)
(diagenetic and catagenetic products of isorenieratenes as biomarkers for photic zone anoxia in petroleum genesis)

RN 187162-60-3 HCAPLUS

CN Acenaphthylene, 5,8-dimethyl-1-[4-methyl-6-(2,3,6-trimethylphenyl)hexyl]-6-(2,3,6-trimethylphenyl)- (9CI) (CA INDEX NAME)



RE.CNT 124 THERE ARE 124 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 11 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1997:38495 HCAPLUS

DN 126:171182

TI Double-bond shifts in [4n]annulenes as a new principle for molecular switches. First results with dimethyl heptalene-1,2- and -4,5-dicarboxylates

AU Briquet, Anne Andree Sophie; Uebelhart, Peter; Hansen, Hans Juergen

CS Organisch-Chemisches Institut, Universitaet Zuerich, Zurich, CH-8057, Switz.

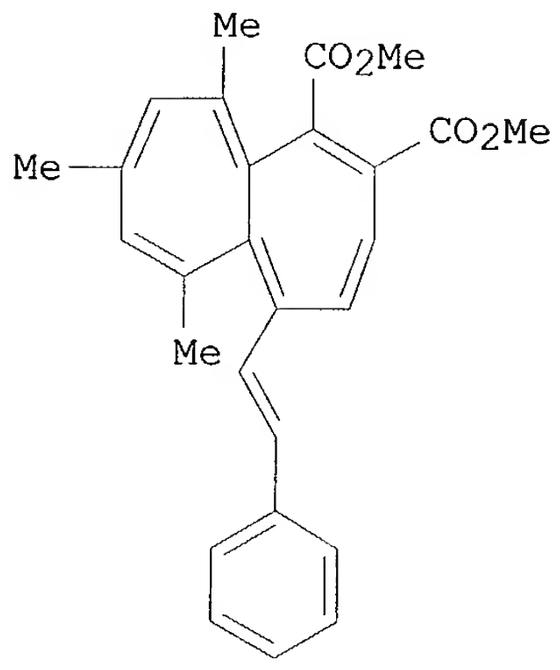
SO Helvetica Chimica Acta (1996), 79(8), 2282-2315
CODEN: HCACAV; ISSN: 0018-019X

PB Verlag Helvetica Chimica Acta

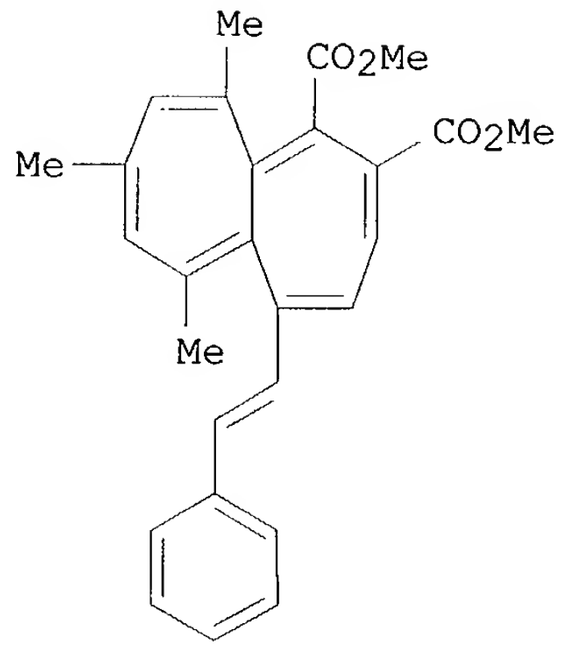
DT Journal

LA English

GI



I



II

AB A concept for mol. switches, based on thermal or photochem. double-bond shifts (DBS) in [4n]annulenes such as heptalenes or cyclooctatetraenes is introduced. Several heptalene-1,2- and -4,5-dicarboxylates with (E)-styryl and Ph groups at C(5) and C(1), or C(4) and C(2), resp., were investigated. X-ray crystal-structure anal. showed that the (E)-styryl group occupies in the crystals an almost perfect s-trans-conformation with respect to the C:C bond of the (E)-styryl moiety and the adjacent C:C bond of the heptalene core. Supplementary 1H-NOE measurements showed that the s-trans-conformations are also adopted in solution Therefore, the DBS process in heptalenes is always accompanied by a 180° torsion of the (E)-styryl group with respect to its adjacent C:C bond of the heptalene core. UV/Vis spectra of the heptalene-1,2- and -4,5-dicarboxylates illustrated that it can be differentiated between an 'off-state', which possesses no 'through-conjugation' of the π-donor substituent and the corresponding MeO2C group and an 'on-state' where this 'through-conjugation' is realized. The 'through-conjugation', i.e., conjugative interaction via the involved s-cis-butadiene substructure of the heptalene skeleton, is indicated by a strong enhancement of the intensities of the heptalene absorption bands I and II. The most impressive examples are the heptalenedicarboxylates I, representing the off-state, and II which stands for the on-state.

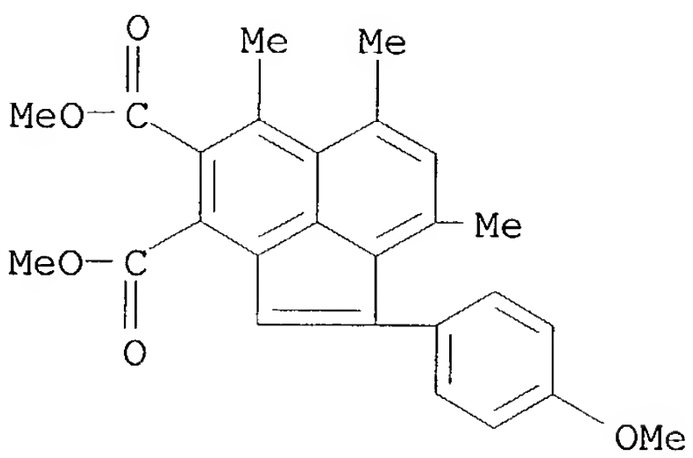
CC 22-6 (Physical Organic Chemistry)
Section cross-reference(s): 24, 25, 75

IT 58151-01-2P 186651-16-1P 186651-17-2P 186651-18-3P
186651-19-4P
RL: BYP (Byproduct); PREP (Preparation)
(preparation of heptalenedicarboxylates)

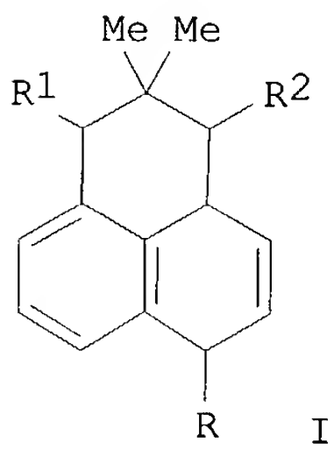
IT **186651-19-4P**
RL: BYP (Byproduct); PREP (Preparation)
(preparation of heptalenedicarboxylates)

RN 186651-19-4 HCAPLUS

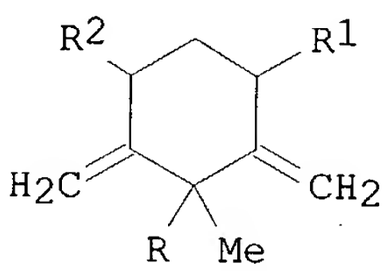
CN 3,4-Acenaphthylenedicarboxylic acid, 1-(4-methoxyphenyl)-5,6,8-trimethyl-, dimethyl ester (9CI) (CA INDEX NAME)



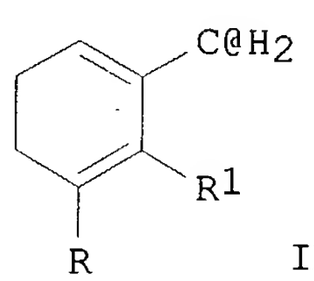
L53 ANSWER 12 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:743463 HCAPLUS
DN 126:131099
TI Resonance energy of diradicals. 1,8-Naphthoquinodimethane
AU Roth, Wolfgang R.; Unger, Christian; Wasser, Thorsten
CS Fakultaet Chemie, Universitaet Bochum, Bochum, D-44780, Germany
SO Liebigs Annalen (1996), (12), 2155-2169
CODEN: LANAEM; ISSN: 0947-3440
PB VCH
DT Journal
LA German
GI



I



II



III

AB From the racemization of methanoacenaphthylene I (R = Me, R1R2 = bond) and the temperature and NO dependence of the trapping rate of perinaphthadiyl I (R = H; R1, R2 = electron) between 218 and 288° the energy profile for the equilibrium I (R = H, R1R2 = bond) .dblarw. I (R = H; R1, R2 = electron) was derived. The singlet-triplet splitting of the diradical is 2.5 kcal·mol-1 with the triplet being the ground state. By comparison of the exptl. reaction enthalpy with the analogous value for bicyclohexane II (R = Me, Et; R1R2 = bond), diradical II (R = Me, Et; R1, R2 = electron) or a hypothetical model reaction with non-interacting radicals the stabilizing interaction of the radicals in the singlet state of I (R = H; R1, R2 = electron) is negligible making the stabilization of the triplet equivalent to the singlet-triplet splitting. By using literature data it is shown by an analogous anal. that the interaction of the radicals in the bisallyl diradical III (R = H, R1 = C•H2) and in the triplet state of III (R = C•H2, R1 = H) is also negligible whereas in the singlet state of III (R = C•H2, R1 = H) the interaction is strongly destabilizing.
CC 22-6 (Physical Organic Chemistry)

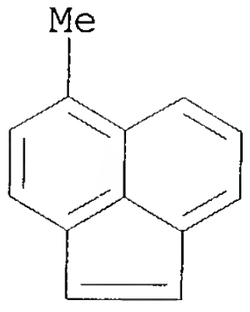
KATHLEEN FULLER EIC 1700 REMSEN 4B28 571/272-2505

Section cross-reference(s): 25

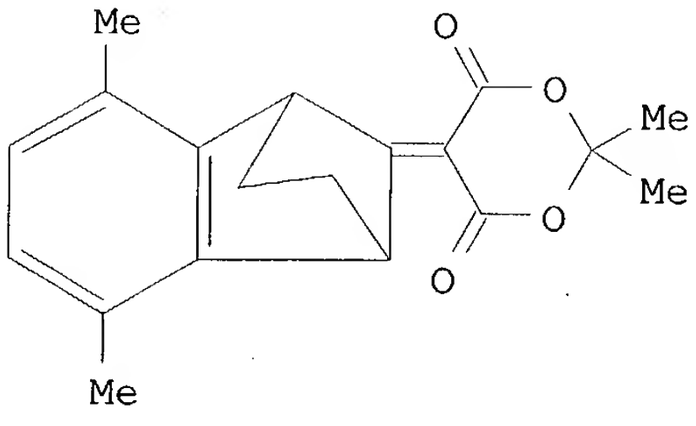
IT 1193-55-1P, 2-Methyl-1,3-cyclohexanedione 19335-98-9P 19345-88-1P
19345-91-6P 19565-21-0P 25112-82-7P 25178-74-9P
41791-10-0P 186349-16-6P 186349-19-9P 186349-26-8P 186349-32-6P
186349-33-7P 186352-69-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(resonance energy of naphthoquinodimethane diradicals)

IT **19345-91-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(resonance energy of naphthoquinodimethane diradicals)

RN 19345-91-6 HCAPLUS
CN Acenaphthylene, 5-methyl- (8CI, 9CI) (CA INDEX NAME)



L53 ANSWER 13 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1994:700262 HCAPLUS
DN 121:300262
TI Conversion of 5-(4,7-dimethyl-1,3-dihydro-1,3-ethano-2H-inden-2-ylidene)-2,2-dimethyl-1,3-dioxan-4,6-dione into 3-methylacenaphthylene in a flash vacuum pyrolytic experiment
AU Bell, Stephanie E. V.; Brown, Roger F. C.; Coulston, Karen J.; Eastwood, Frank W.
CS Chemistry Department, Monash University, Clayton, 3168, Australia
SO Australian Journal of Chemistry (1994), 47(8), 1469-81
CODEN: AJCHAS; ISSN: 0004-9425
DT Journal
LA English
GI



I

AB Flash vacuum pyrolysis of 5-(4,7-dimethyl-1,3-dihydro-1,3-ethano-2H-inden-2-ylidene)-2,2-dimethyl-1,3-dioxan-4,6-dione (I) at temps. in the range 600-750° led to complex mixts., but at higher temps. (850°)

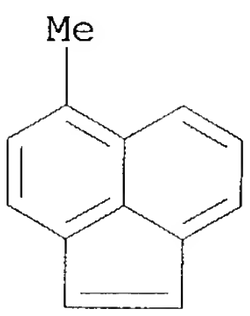
it was converted into 3-methylacenaphthylene (major) and 1,4-dimethylnaphthalene (minor). 5-Ethenyl-1,4-dimethylnaphthalene on f.v.p. at 850° gave 5-methylacenaphthylene together with other compds. and was not on the reaction pathway.

CC 22-4 (Physical Organic Chemistry)
Section cross-reference(s): 25

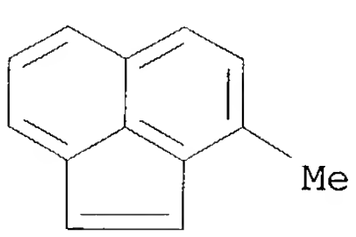
IT **19345-91-6P**, 5-Methylacenaphthylene **19345-94-9P**, 3-Methylacenaphthylene 88916-64-7P, 5-Ethenyl-1,4-dimethylnaphthalene 159263-64-6P 159263-65-7P 159263-66-8P 159263-69-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(study of pyrolysis/carbene rearrangement of (ethanoindenylidene)-1,3-dioxanedione)

IT **19345-91-6P**, 5-Methylacenaphthylene **19345-94-9P**, 3-Methylacenaphthylene
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(study of pyrolysis/carbene rearrangement of (ethanoindenylidene)-1,3-dioxanedione)

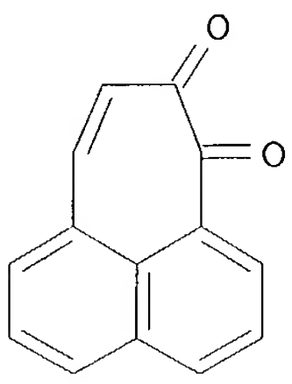
RN 19345-91-6 HCAPLUS
CN Acenaphthylene, 5-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 19345-94-9 HCAPLUS
CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)



L53 ANSWER 14 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1994:579005 HCAPLUS
DN 121:179005
TI Some physical properties of methyl derivatives of o-pleiadienequinones
AU Ohashi, Akihiro; Aida, Takashi; Tsunetsugu, Josuke
CS Department of Chemistry, Faculty of Science, Saitama University, Urawa, 338, Japan
SO Journal of Molecular Structure (1994), 324(1-2), 75-82
CODEN: JMOSB4; ISSN: 0022-2860
DT Journal
LA English
GI



I

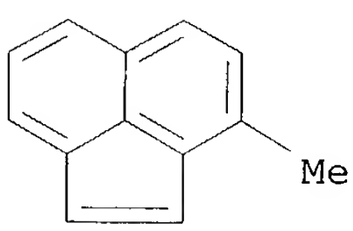
AB Spectral (UV, IR, mass, 1H and 13C NMR) and electrochem. properties of o-pleiadienequinone (I) and its Me derivs. are described. Heats of formation are calculated by the MNDO-PM3 method.

CC 22-10 (Physical Organic Chemistry)
Section cross-reference(s): 72

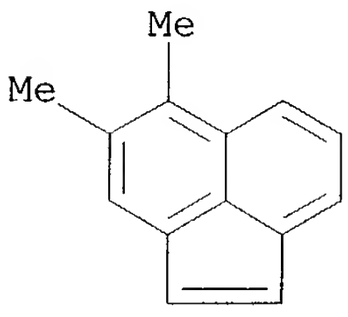
IT **19345-94-9P**, 3-Methylacenaphthylene **41002-81-7P**, 4,5-Dimethylacenaphthylene **41002-83-9P**, 5,6-Dimethylacenaphthylene **41082-61-5P**, 3,7-Dimethylacenaphthylene
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cycloaddn. reaction with dichloroketene)

IT **19345-94-9P**, 3-Methylacenaphthylene **41002-81-7P**, 4,5-Dimethylacenaphthylene **41002-83-9P**, 5,6-Dimethylacenaphthylene **41082-61-5P**, 3,7-Dimethylacenaphthylene
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cycloaddn. reaction with dichloroketene)

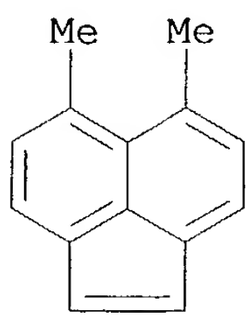
RN 19345-94-9 HCAPLUS
CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)



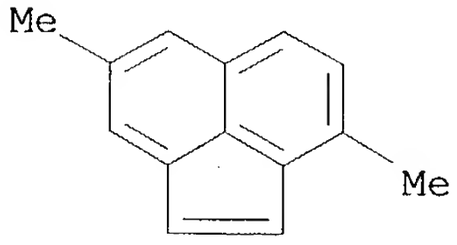
RN 41002-81-7 HCAPLUS
CN Acenaphthylene, 4,5-dimethyl- (9CI) (CA INDEX NAME)



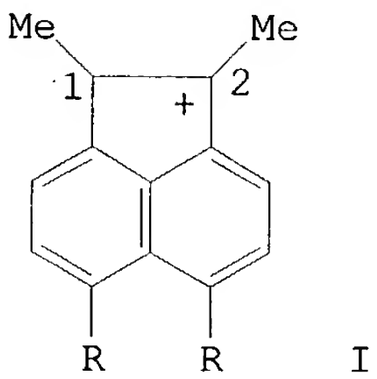
RN 41002-83-9 HCAPLUS
CN Acenaphthylene, 5,6-dimethyl- (6CI, 9CI) (CA INDEX NAME)



RN 41082-61-5 HCAPLUS
CN Acenaphthylene, 3,7-dimethyl- (9CI) (CA INDEX NAME)



L53 ANSWER 15 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1991:582355 HCAPLUS
DN 115:182355
TI General structure-reactivity relationships for 1,2-hydrogen shifts in carbocations and neutral compounds
AU Borodkin, G. I.; Susharin, E. R.; Elanov, I. R.; Shakirov, M. M.; Shubin, V. G.
CS Novosib. Inst. Org. Khim., Novosibirsk, USSR
SO Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1991), (6), 1352-8
CODEN: IASKA6; ISSN: 0002-3353
DT Journal
LA Russian
GI



I

AB Linear equations correlating the activation parameters for degenerate 1,2 H shift in acenaphthylenonium ions I (R = Me, Br) with chemical shift of the carbonium-ion C or other measures of electron deficit - total or π-electron charge at the carbonium C calculated by CNDO/2 - were established.

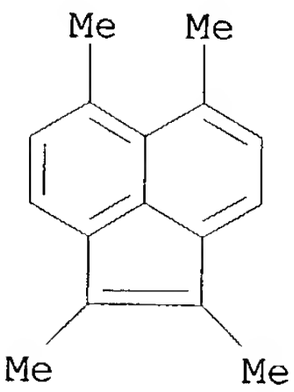
CC 22-6 (Physical Organic Chemistry)
IT 132118-72-0 **132118-73-1**

KATHLEEN FULLER EIC 1700 REMSEN 4B28 571/272-2505

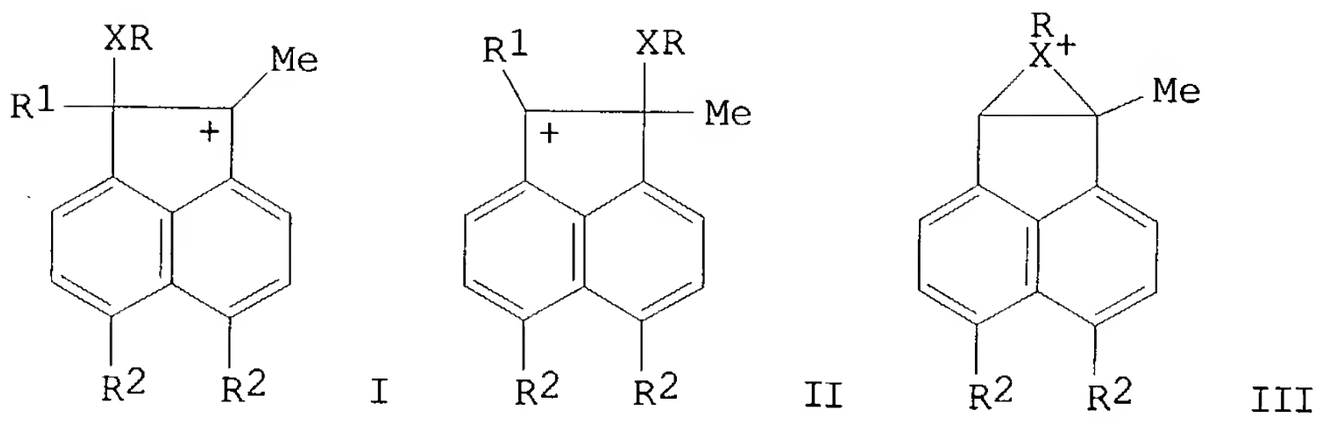
RL: RCT (Reactant); RACT (Reactant or reagent)
(protonation of, in superacid, carbonium ion by)

IT **132118-73-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(protonation of, in superacid, carbonium ion by)

RN 132118-73-1 HCAPLUS
CN Acenaphthylene, 1,2,5,6-tetramethyl- (9CI) (CA INDEX NAME)

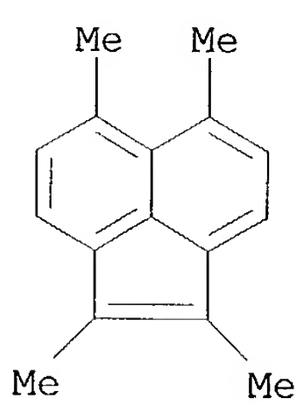


L53 ANSWER 16 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1991:100774 HCAPLUS
DN 114:100774
TI Stereoelectronic aspects of the interaction between reagents RXCl (X = sulfur, selenium) and acenaphthylene derivatives in superacids
AU Borodkin, G. I.; Chernyak, E. I.; Shakirov, M. M.; Shubin, V. G.
CS Novosib. Inst. Org. Khim., Novosibirsk, USSR
SO Metalloorganicheskaya Khimiya (1990), 3(5), 1017-24
CODEN: MEKHEX; ISSN: 0235-0114
DT Journal
LA Russian
GI



AB Substituent effects on the relative equilibrium stability of acynaphthylenonium ions I, II and π-complex III (RX = MeS, C6H5S, C6F5S, C6H5Se, C6F5Se, OH, Br; R1 = Me, CH2Cl; R2 = H, Br, Me) were studied by NMR. The relative contribution of III falls with increasing atomic number of X, electron-donor character of R1, and electron-accepting character of R2. In several of the episulfonium ions III, trans stereochem. of the R and R1 groups was established by NMR and interpreted as a steric effect; the absence of temperature effect on the NMR indicated that these trans isomers were static, and that a rapid equilibrium with minor concentration of the cis isomer is not

involved. MINDO/3 calcns. on the potential energy surface of III are reported as well.
CC 22-4 (Physical Organic Chemistry)
IT 132118-72-0P **132118-73-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion of, to acynaphthylenonium ion)
IT **132118-73-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion of, to acynaphthylenonium ion)
RN 132118-73-1 HCAPLUS
CN Acenaphthylene, 1,2,5,6-tetramethyl- (9CI) (CA INDEX NAME)

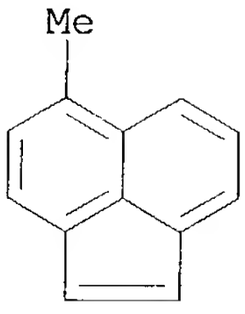


L53 ANSWER 17 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:575325 HCAPLUS
DN 113:175325
TI Hydropyrolysis of coal. Influence of temperature and hydrogen pressure on the yield and composition of hydropyrolysis tars
AU Kaernbach, W.; Dyla, P.; Zobel, H.
CS Inst. Coal Chem., Pol. Acad. Sci., Gliwice, Pol.
SO Erdoel & Kohle, Erdgas, Petrochemie (1990), 43(7/8), 291-4
CODEN: EKEPAB; ISSN: 0014-0058
DT Journal
LA German
AB The influence of reaction conditions on the hydropyrolysis of Polish hard coals is described. The yield of the main products and the composition of the structure types of the hydropyrolysis tars were studied by TGA and gas chromatog. The hydropyrolysis was carried out in a fixed-bed pressure reactor. The optimal reaction conditions were at 873 K and 3 MPa H pressure.
CC 51-21 (Fossil Fuels, Derivatives, and Related Products)
IT 71-43-2P, Benzene, preparation 90-12-0P, 1-Methylnaphthalene 91-20-3P, Naphthalene, preparation 91-57-6P, 2-Methylnaphthalene 92-52-4P, 1,1'-Biphenyl, preparation 95-47-6P, preparation 95-63-6P, 1,2,4-Trimethylbenzene 100-41-4P, Ethylbenzene, preparation 106-42-3P, p-Xylene, preparation 108-38-3P, m-Xylene, preparation 108-67-8P, 1,3,5-Trimethylbenzene, preparation 108-88-3P, preparation 111-65-9P, N-Octane, preparation 111-66-0P, 1-Octene 111-84-2P, Nonane 112-40-3P, n-Dodecane 112-41-4P, 1-Dodecene 112-88-9P, 1-Octadecene 112-95-8P, n-Eicosane 124-11-8P, 1-Nonene 124-18-5P, n-Decane 142-82-5P, n-Heptane, preparation 496-11-7P, Indan 526-73-8P, 1,2,3-Trimethylbenzene 538-68-1P, Pentylbenzene 544-76-3P, n-Hexadecane 571-58-4P, 1,4-Dimethylnaphthalene 573-98-8P, 1,2-Dimethylnaphthalene 575-37-1P, 1,7-Dimethylnaphthalene 575-41-7P, 1,3-Dimethylnaphthalene 575-43-9P, 1,6-Dimethylnaphthalene 581-40-8P, 2,3-Dimethylnaphthalene 581-42-0P, 2,6-Dimethylnaphthalene 582-16-1P, 2,7-Dimethylnaphthalene 593-45-3P, n-Octadecane 593-49-7P,

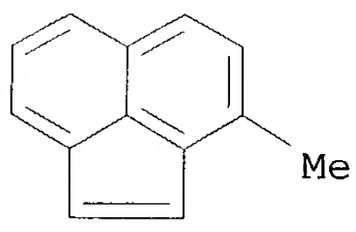
n-Heptacosane 629-50-5P, n-Tridecane 629-59-4P, n-Tetradecane 629-62-9P, Pentadecane 629-78-7P, n-Heptadecane 629-92-5P, n-Nonadecane 629-94-7P, n-Heneicosane 629-97-0P, n-Docosane 629-99-2P, n-Pentacosane 630-01-3P, n-Hexacosane 630-02-4P, n-Octacosane 630-03-5P, n-Nonacosane 630-04-6P, n-Hentriacontane 638-67-5P, n-Tricosane 638-68-6P, n-Triacontane 641-91-8P, 1,2,5-Trimethylnaphthalene 646-31-1P, n-Tetracosane 767-58-8P, 1-Methylindan 821-95-4P, 1-Undecene 824-22-6P, 4-Methylindan 824-63-5P, 2-Methylindan 829-26-5P, 2,3,6-Trimethylnaphthalene 872-05-9P, 1-Decene 874-35-1P, 5-Methylindan 939-27-5P, 2-Ethylnaphthalene 1120-21-4P, Undecane 1127-76-0P, 1-Ethylnaphthalene 1320-27-0P, Pentylnaphthalene 1599-67-3P, 1-Docosene 1680-51-9P 1685-83-2P 2131-38-6P, 1,3,7-Trimethylnaphthalene 2131-39-7P, 1,3,5-Trimethylnaphthalene 2131-42-2P, 1,4,6-Trimethylnaphthalene 2245-38-7P, 2,3,5-Trimethylnaphthalene 2437-56-1P, 1-Tridecene 2717-42-2P, 1,2,4-Trimethylnaphthalene 2809-64-5P 3031-08-1P, 1,3,6-Trimethylnaphthalene 4471-17-4P, Methyldiphenyl 13556-58-6P 18435-45-5P, 1-Nonadecene **19345-91-6P 19345-94-9P 19345-97-2P** 26266-05-7P, n-Heptadecene 26916-61-0P 26952-13-6P, n-Tetradecene 26952-14-7P, n-Hexadecene 27251-68-9P, n-Pentadecene 27378-74-1P, Propylnaphthalene 27400-78-8P, n-Eicosene 27400-79-9P, n-Heneicosene 31324-50-2P 31391-42-1P 31711-50-9P, Butylnaphthalene 36541-18-1P, Trimethylindan 51855-29-9P 53563-67-0P, Dimethylindan 56924-46-0P, n-Tricosene 66256-38-0P, 4-Ethylindan 95012-76-3P 95676-53-2P 108114-27-8P 130004-87-4P 130004-89-6P 130005-08-2P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in hydropyrolysis tars of Polish coal)

IT **19345-91-6P 19345-94-9P 19345-97-2P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in hydropyrolysis tars of Polish coal)

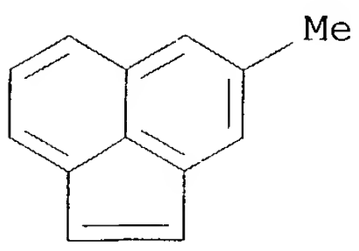
RN 19345-91-6 HCAPLUS
CN Acenaphthylene, 5-methyl- (8CI, 9CI) (CA INDEX NAME)



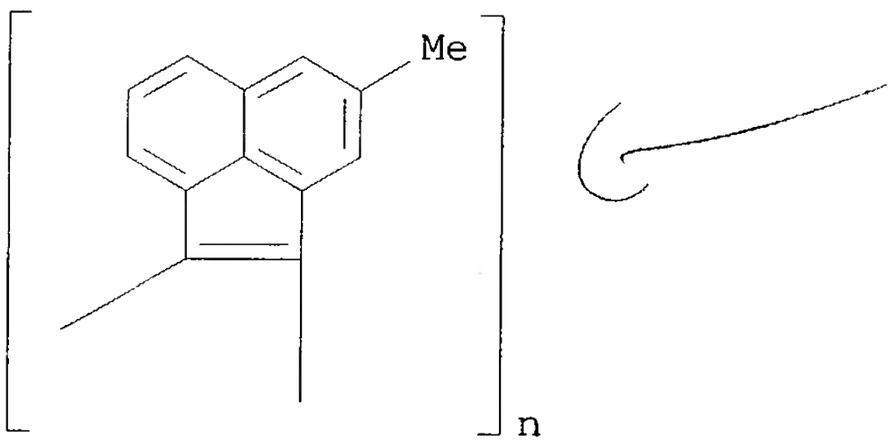
RN 19345-94-9 HCAPLUS
CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 19345-97-2 HCAPLUS
CN Acenaphthylene, 4-methyl- (8CI, 9CI) (CA INDEX NAME)



L53 ANSWER 18 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1987:637616 HCAPLUS
DN 107:237616
TI Structure and properties of nonclassical polymers. V. On a class of nonalternant polymers with localized nonbonding bands
AU Polansky, O. E.; Schuster, P.; Ivanov, Ts.; Tyutyulkov, N.
CS Max-Planck-Inst. Strahlenchem., Muelheim an der Ruhr, D-4330, Fed. Rep. Ger.
SO International Journal of Quantum Chemistry (1987), 32(4), 491-9
CODEN: IJQCB2; ISSN: 0020-7608
DT Journal
LA English
AB Nonclassical, extended polymeric hydrocarbon networks exhibiting localized, infinitely narrow nonbonding bands (NBMO) owing to different structural peculiarities were studied, and proof of the rigorous localization of the occurring NBMOs was provided. The possible ferromagnetic alignment originating from the spin correlation in this band is discussed. A specific relevance of the Coulson-Rushbrrok theorem to nonalternant polymers was realized on the basis of the structural principles formulated, which included dividing the monomeric unit into a nonclassical alternant fragment (Q) (e.g., pentadienyl) and a classical subunit (R) (e.g., ethene) and bridging the Q subunits with R subunits.
CC 36-2 (Physical Properties of Synthetic High Polymers)
Section cross-reference(s): 65, 77
IT 111763-22-5 111763-23-6 **111763-24-7**
RL: PRP (Properties)
(with localized nonbonding bands, band structure and magnetic order in relation to)
IT **111763-24-7**
RL: PRP (Properties)
(with localized nonbonding bands, band structure and magnetic order in relation to)
RN 111763-24-7 HCAPLUS
CN Poly(4-methyl-1,2-acenaphthylenediyl) (9CI) (CA INDEX NAME)

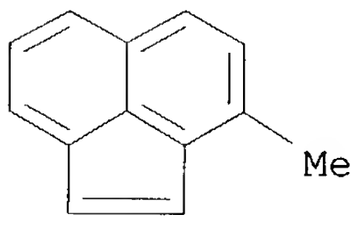


L53 ANSWER 19 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN

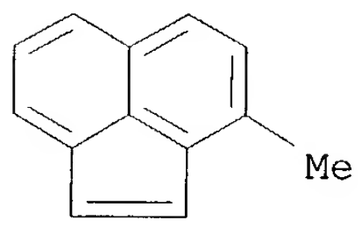
AN 1987:181789 HCAPLUS
DN 106:181789
TI Identification of organic compounds produced during combustion of a polymer mixture
AU Hawley-Fedder, R. A.; Parsons, M. L.; Karasek, F. W.
CS Lawrence Livermore Natl. Lab., Livermore, CA, 94550, USA
SO Journal of Chromatography (1987), 387, 207-21
CODEN: JOCRAM; ISSN: 0021-9673
DT Journal
LA English
AB A mixture containing polyethylene [9002-88-4], polystyrene [9003-53-6], and poly(vinyl chloride) [9002-86-2] was subjected to oxidative thermal degradation at temps. of 800-950°. Break-down products were collected on glass wool or in cold traps for anal. by capillary gas chromatog. and gas chromatog.-mass spectrometry. Combustion products included alkyl benzenes, hydrocarbons, alkenes, biphenyls, and polycyclic aromatic hydrocarbons containing 2-6 rings.
CC 59-2 (Air Pollution and Industrial Hygiene)
Section cross-reference(s): 35, 38, 60
IT 56-49-5P, 3-Methylcholanthrene 56-55-3P, Benzo[a]anthracene 84-15-1P, o-Terphenyl 85-01-8P, preparation 86-73-7P, Fluorene 90-12-0P, 1-Methylnaphthalene 91-20-3P, preparation 91-57-6P, 2-Methylnaphthalene 92-06-8P, m-Terphenyl 92-24-0P, Naphthacene 92-52-4P, preparation 92-94-4P, p-Terphenyl 95-13-6P 98-82-8P, Cumene 100-42-5P, preparation 100-80-1P, m-Methylstyrene 101-81-5P, Diphenylmethane 103-65-1P, Propylbenzene 120-12-7P, Anthracene, preparation 129-00-0P, preparation 135-48-8P, Pentacene 191-24-2P, Benzo[ghi]perylene 191-26-4P, Dibenzo[def,mno]chrysene 195-19-7P, Benzo[c]phenanthrene 203-12-3P, Benzo[ghi]fluoranthene 203-64-5P, 4,5-Methylenephenanthrene 203-80-5P 206-44-0P, Fluoranthene 208-96-8P, Acenaphthylene 213-46-7P, Picene 215-58-7P, Dibenz[a,c]anthracene 217-59-4P, Triphenylene 218-01-9P, Chrysene 275-51-4P, Azulene 300-57-2P, 3-Phenylpropene 496-11-7P, Indane 501-65-5P, Diphenylacetylene 530-48-3P, 1,1-Diphenylethene 575-41-7P, 1,3-Dimethylnaphthalene 588-59-0P 604-53-5P, 1,1'-Binaphthyl 605-02-7P, 1-Phenylnaphthalene 610-48-0P, 1-Methylanthracene 611-15-4P, o-Methylstyrene 611-45-0P, 1-Benzylnaphthalene 612-78-2P, 2,2'-Binaphthyl 612-94-2P, 2-Phenylnaphthalene 613-31-0P, Dihydroanthracene 622-97-9P, p-Methylstyrene 637-50-3P, 1-Propenylbenzene 643-58-3P, 2-Methylbiphenyl 643-93-6P, 3-Methylbiphenyl 644-08-6P, 4-Methylbiphenyl 826-74-4P, 1-Vinylnaphthalene 827-54-3P, 2-Vinylnaphthalene 832-71-3P, 3-Methylphenanthrene 883-20-5P, 9-Methylphenanthrene 939-27-5P, 2-Ethylnaphthalene 1081-75-0P, 1,3-Diphenylpropane 1127-76-0P, 1-Ethylnaphthalene 1430-97-3P, 2-Methylfluorene 1730-37-6P, 1-Methylfluorene 2381-21-7P, 1-Methylpyrene 2489-87-4P 2498-75-1P 2498-77-3P 2523-37-7P, 9-Methylfluorene 2871-91-2P 3351-30-2P, 4-Methylchrysene 4325-74-0P, 1,2'-Binaphthyl 4325-76-2P, 1-Phenylphenanthrene 6111-78-0P **19345-94-9P**, 3-Methylacenaphthylene 19345-99-4P, 1-Methylacenaphthylene 25323-41-5P, Chloroxylene 25550-14-5P, Methylethylbenzene 26856-35-9P, Dihydrophenanthrene 28700-83-6P 29036-02-0P, Quaterphenyl 30777-18-5P, Benzo[a]fluorene 30777-19-6P, Benzo[b]fluorene 30900-94-8P 38620-92-7P, Benzylnaphthalene 56832-73-6P, Benzofluoranthene 66161-17-9P 73467-76-2P, Benzopyrene 107843-54-9P 108115-36-2P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in combustion of polyethylene-polystyrene-poly(vinyl chloride) mixts., waste incineration in relation to)

KATHLEEN FULLER EIC 1700 REMSEN 4B28 571/272-2505

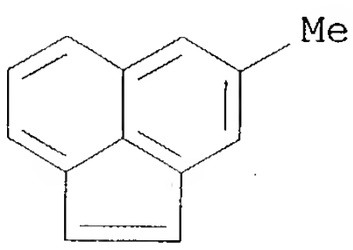
IT **19345-94-9P**, 3-Methylacenaphthylene
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in combustion of polyethylene-polystyrene-poly(vinyl chloride) mixts., waste incineration in relation to)
RN 19345-94-9 HCAPLUS
CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)



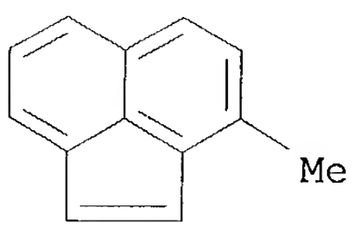
L53 ANSWER 20 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1985:154078 HCAPLUS
DN 102:154078
TI Products obtained during combustion of polymers under simulated incinerator conditions. III. Poly(vinyl chloride)
AU Hawley-Fedder, R. A.; Parsons, M. L.; Karasek, F. W.
CS Dep. Chem., Arizona State Univ., Tempe, AZ, 85287, USA
SO Journal of Chromatography (1984), 315, 211-21
CODEN: JOCRAM; ISSN: 0021-9673
DT Journal
LA English
AB Combustion products from poly(vinyl chloride) [9002-86-2] were determined using gas chromatog. and gas chromatog.-mass spectrometry. Combustion conditions were 800-950°, and an attempt was made to approx. municipal incinerator conditions. Compds. identified consisted of PAHs and alkylbenzenes. Two chlorinated species were identified.
CC 59-4 (Air Pollution and Industrial Hygiene)
Section cross-reference(s): 38
IT 50-32-8P, preparation 56-49-5P 56-55-3P 71-43-2P, preparation
85-01-8P, preparation 86-73-7P 90-12-0P 91-20-3P, preparation
91-57-6P 92-52-4P, preparation 92-94-4P 95-13-6P 103-65-1P
108-95-2P, preparation 120-12-7P, preparation 129-00-0P, preparation
135-48-8P 191-24-2P 192-97-2P 195-19-7P 198-55-0P 203-12-3P
203-64-5P 203-80-5P 206-44-0P 208-96-8P 213-46-7P 218-01-9P
275-51-4P 501-65-5P 571-58-4P 575-41-7P 581-40-8P 581-42-0P
605-02-7P 612-94-2P 613-12-7P 643-93-6P 644-08-6P 826-74-4P
827-54-3P 883-20-5P 886-66-8P 1127-76-0P 1430-97-3P 1576-69-8P
1705-85-7P 1730-37-6P 2381-21-7P 2381-31-9P 2417-82-5P
2498-77-3P 2871-91-2P 3287-02-3P 3351-31-3P 4325-76-2P
6111-78-0P 6268-37-7P 17088-22-1P **19345-94-9P**
19345-97-2P 19345-99-4P 25323-41-5P 26856-35-9P
30777-18-5P 30777-19-6P 42862-12-4P 53571-97-4P 56832-73-6P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from polyvinyl chloride incineration)
IT **19345-94-9P 19345-97-2P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from polyvinyl chloride incineration)
RN 19345-94-9 HCAPLUS
CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 19345-97-2 HCAPLUS
CN Acenaphthylene, 4-methyl- (8CI, 9CI) (CA INDEX NAME)



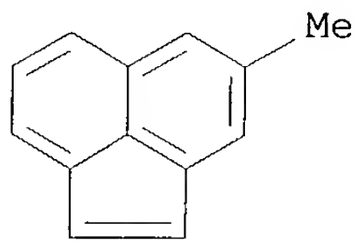
L53 ANSWER 21 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1985:66681 HCAPLUS
DN 102:66681
TI Products obtained during combustion of polymers under simulated incinerator conditions. I. Polyethylene
AU Hawley-Fedder, R. A.; Parsons, M. L.; Karasek, F. W.
CS Dep. Chem., Arizona State Univ., Tempe, AZ, 85287, USA
SO Journal of Chromatography (1984), 314, 263-73
CODEN: JOCRAM; ISSN: 0021-9673
DT Journal
LA English
AB An apparatus permitting the combustion of large (2 g) polymer samples at high temperature is described. Effluents from combustion are collected in cold traps (liquid N) and on glass wool for anal. by capillary gas chromatog. and gas chromatog.-mass spectrometry. Products from polyethylene [9002-88-4] combustion at 800, 850, 900, and 950° are determined
CC 59-4 (Air Pollution and Industrial Hygiene)
Section cross-reference(s): 38
IT **19345-94-9 19345-97-2** 19345-99-4 30777-18-5
30777-19-6 35465-71-5
RL: OCCU (Occurrence)
(in polyethylene incineration combustion products)
IT **19345-94-9 19345-97-2**
RL: OCCU (Occurrence)
(in polyethylene incineration combustion products)
RN 19345-94-9 HCAPLUS
CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 19345-97-2 HCAPLUS

KATHLEEN FULLER EIC 1700 REMSEN 4B28 571/272-2505

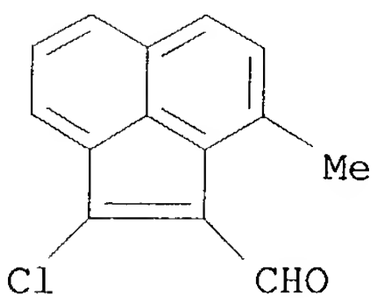
CN Acenaphthylene, 4-methyl- (8CI, 9CI) (CA INDEX NAME)



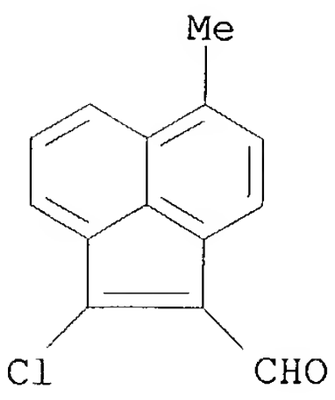
L53 ANSWER 22 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1982:438636 HCAPLUS
DN 97:38636
TI Anomalous Leuckart reaction of acenaphthenones. II. Anomalous Leuckart reaction of 3-methyl- and 5-methyl-1-acenaphthenones
AU Tatsugi, Jiro; Okumura, Michio
CS Dep. Appl. Chem., Aichi Inst. Technol., Toyota, 470-03, Japan
SO Nippon Kagaku Kaishi (1982), (5), 876-9
CODEN: NKAKB8; ISSN: 0369-4577
DT Journal
LA Japanese
OS CASREACT 97:38636
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Methylacenaphthenone isomers (I; R = Me, R1 = H, R1 = H, R = H, R1 = Me) gave anomalous Leuckart reaction products II and III, together with formylamino derivs. (IV). The aldol-type condensation products (V) were obtained from I (R = R1 = H; R = H, R1 = Me) but not from I (R = Me, R1 = H).
CC 25-26 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT **58231-30-4P** 82318-84-1P 82318-85-2P 82318-86-3P
82318-87-4P 82318-88-5P 82318-89-6P 82325-54-0P **82375-05-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **58231-30-4P 82375-05-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 58231-30-4 HCAPLUS
CN 1-Acenaphthylenecarboxaldehyde, 2-chloro-8-methyl- (9CI) (CA INDEX NAME)



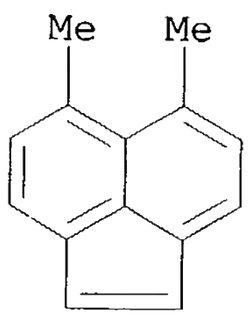
RN 82375-05-1 HCAPLUS
CN 1-Acenaphthylenecarboxaldehyde, 2-chloro-6-methyl- (9CI) (CA INDEX NAME)



L53 ANSWER 23 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1981:588459 HCAPLUS
DN 95:188459
TI Radiation-resistant polymer compositions
PA Japan Atomic Energy Research Institute, Japan; Furukawa Electric Co., Ltd.
SO Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 56084748	A2	19810710	JP 1979-161570	19791214
	JP 61011263	B4	19860402		
PRAI	JP 1979-161570		19791214		

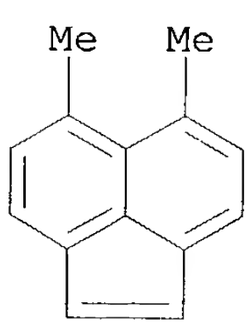
AB Thermoplastic and rubber compns. with improved radiation resistance contain a C1-4 alkyl- or haloacenaphthylene and/or a haloindene ≥0.5, a hydroperoxide 0.2-10, and an organic peroxide 0.5-10 phr. For example, a vulcanizate from 60:40 ethylene-propene rubber 100, Nocrack 224 0.5, S 0.1, clay 100, dicumyl peroxide 1, tert-Bu hydroperoxide 3, and 5,6-dimethylacenaphthylene (I) [**41002-83-9**] 3 parts had tensile strength 0.66 kg/mm2 (0.69 kg/mm2 after 100 Mrads γ-ray irradiation) and elongation 690 (610)%, compared with 0.65 (0.45) and 680 (140), resp., for a control not containing I.
IC C08L101-00; C08K005-01; C08K005-03; C08K005-14
CC 38-9 (Elastomers, Including Natural Rubber)
IT **41002-83-9**
RL: USES (Uses)
(ethylene-propene rubber containing, radiation-resistant)
IT **41002-83-9**
RL: USES (Uses)
(ethylene-propene rubber containing, radiation-resistant)
RN 41002-83-9 HCAPLUS
CN Acenaphthylene, 5,6-dimethyl- (6CI, 9CI) (CA INDEX NAME)



L53 ANSWER 24 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1981:588151 HCAPLUS
DN 95:188151
TI Fireproofing of polymers
PA Japan Atomic Energy Research Institute, Japan; Furukawa Electric Co., Ltd.
SO Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 56084731	A2	19810710	JP 1979-161572	19791214
	JP 60015655	B4	19850420		
PRAI	JP 1979-161572		19791214		

AB Loss of strength in fireproofing of polymers with halogen compds. is reduced by crosslinking the fireproofed polymers with >0.5 phr acenaphthylene, optionally containing C1-4 alkyl or halogen groups, or chlorinated or brominated indenes. For example, a 1-mm sheet of polyethylene [9002-88-4] 100, Nocrack 300 0.3, (C6Br5)2O [1163-19-5] 30, Sb2O3 10, and 5,6-dimethylacenaphthylene (I) [**41002-83-9**] 10 parts was irradiated with 20 Mrad electron beams to give a crosslinked sheet with tensile strength 1.51 kg/mm2, elongation 360%, and O index 25.5, compared with 1.22, 290, and 24.0, resp., without I, and 2.27, 480, and 19.0, resp., for polyethylene containing 0.3 phr Nocrack 300.
IC C08J007-12; C08K005-01; C08K005-03; C08L101-00
CC 36-6 (Plastics Manufacture and Processing)
IT **41002-83-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(crosslinking by, of fireproofed polyethylene for strength retention)
IT **41002-83-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(crosslinking by, of fireproofed polyethylene for strength retention)
RN 41002-83-9 HCAPLUS
CN Acenaphthylene, 5,6-dimethyl- (6CI, 9CI) (CA INDEX NAME)



L53 ANSWER 25 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1981:570432 HCAPLUS
DN 95:170432
TI Chlorine-containing resin compositions
PA Japan Atomic Energy Research Institute, Japan; Furukawa Electric Co., Ltd.
SO Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

PI	JP 56084730	A2	19810710	JP 1979-161571	19791214
	JP 60014779	B4	19850416		
PRAI	JP 1979-161571		19791214		

AB Cl-containing polymers modified with ≥0.5 phr C1-4 alkyl or halo acenaphthalenes and/or haloindenes under electron beam irradiation showed reduced HCl evolution in combustion. Thus, a 1 mm sheet from PVC [9002-86-2] 100, DOP 50, tribase 5, dibasic Pb stearate 0.3, CaCO3 70, and 5,6-dimethylacenaphthylene (I) [**41002-83-9**] 5 parts was irradiated with 15 Mrads electron beam to give a specimen with tensile strength 1.53 kg/mm2, elongation 260%, tensile strength retention (after 4 h in 70° oil) 94%, elongation retention 83%, and HCl evolution 60 mg/g, compared with 2.10, 350, 105, 90, and 285, resp., for a control without I and the irradiation and 1.10, 170, 73, 53, and 60, resp., for a control without I, but with the irradiation

IC C08J007-12; C08K003-22; C08K003-26; C08K005-01

CC 36-6 (Plastics Manufacture and Processing)

IT **41002-83-9**

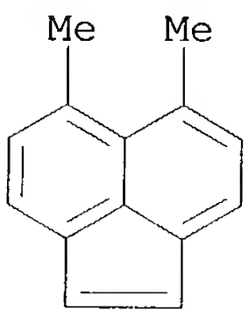
RL: USES (Uses)
(PVC containing, electron beam-irradiated, with improved hydrogen chloride evolution resistance)

IT **41002-83-9**

RL: USES (Uses)
(PVC containing, electron beam-irradiated, with improved hydrogen chloride evolution resistance)

RN 41002-83-9 HCAPLUS

CN Acenaphthylene, 5,6-dimethyl- (6CI, 9CI) (CA INDEX NAME)



L53 ANSWER 26 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1981:498826 HCAPLUS

DN 95:98826

TI Fireproofing agents

PA Japan Atomic Energy Research Institute, Japan

SO Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF

DT Patent

LA Japanese

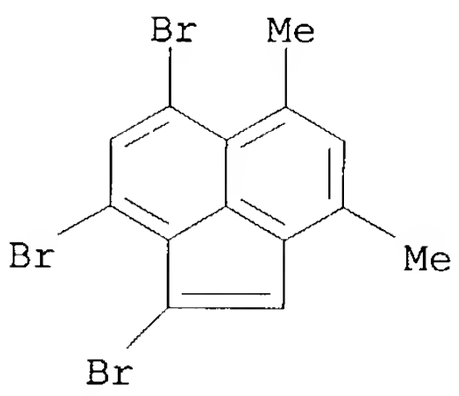
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 56016511	A2	19810217	JP 1979-92019	19790719
	JP 58001146	B4	19830110		
	US 4289687	A	19810915	US 1980-114420	19800122
PRAI	JP 1979-4802		19790122		
	JP 1979-92019		19790719		

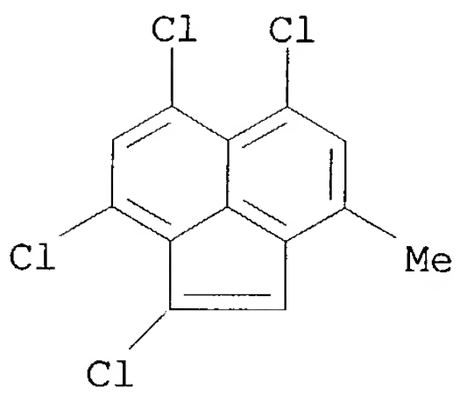
AB A fire-resistant resin composition contains an acenaphthylene derivative with 2-7
Cl and/or Br atoms and 1-4 C1-4 alkyl, alkoxy, and/or alkyl ester groups,

and is treated to generate free radicals. Thus, to polyethylene (I) (ZF-30) [9002-88-4] 100, chlorinated I (Cl content 40%) 35, 3-methyl-1,5,6,8-tetrabromoacenaphthylene [**78536-16-0**] 30, Sb2O3 20, and 2,6-di-tert-butylphenol 0.5 part mixed by a 120°-heat roller, 3 parts dicumyl peroxide [80-43-3] was added at 20-70°, and the mixture was hot-pressed at 160° for 30 min to form 1- or 3-mm-thick sheets. No bloom appeared on a sample kept in a 121° bath for 168 h and cooled to room temperature Burning time (ASTM D 635-74) before and after the blooming test was unchanged at 4 s. The sample had O index 30% and residual fire-retardant (after Soxhlet extraction) 72%.

IC C08F291-00; C08F002-44; C08K005-03
CC 36-6 (Plastics Manufacture and Processing)
IT **78536-19-3** 78536-20-6
RL: USES (Uses)
(fireproofing agents, for EPDM rubber)
IT **78536-18-2**
RL: USES (Uses)
(fireproofing agents, for ethylene-vinyl acetate copolymer)
IT **78536-16-0** 78536-17-1
RL: USES (Uses)
(fireproofing agents, for polyethylene)
IT **78536-19-3**
RL: USES (Uses)
(fireproofing agents, for EPDM rubber)
RN 78536-19-3 HCAPLUS
CN Acenaphthylene, 1,6,8-tribromo-3,5-dimethyl- (9CI) (CA INDEX NAME)



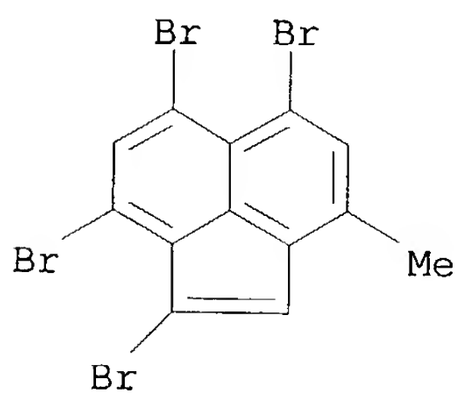
IT **78536-18-2**
RL: USES (Uses)
(fireproofing agents, for ethylene-vinyl acetate copolymer)
RN 78536-18-2 HCAPLUS
CN Acenaphthylene, 1,5,6,8-tetrachloro-3-methyl- (9CI) (CA INDEX NAME)



IT **78536-16-0**
RL: USES (Uses)

KATHLEEN FULLER EIC 1700 REMSEN 4B28 571/272-2505

(fireproofing agents, for polyethylene)
RN 78536-16-0 HCAPLUS
CN Acenaphthylene, 1,5,6,8-tetrabromo-3-methyl- (9CI) (CA INDEX NAME)



L53 ANSWER 27 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1981:31904 HCAPLUS
DN 94:31904
TI Polymers and rubbers with good resistance to radiochemical degradation
PA Japan Atomic Energy Research Institute, Japan
SO Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

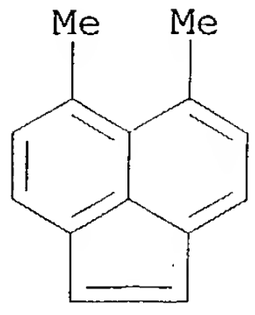
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 55106228	A2	19800814	JP 1979-4803	19790122
	JP 61050490	B4	19861105		
PRAI	JP 1979-4803		19790122		

AB Thermoplastic polymers or rubbers containing radical initiators and >0.5 weight percent (based on polymers) acenaphthylene derivs. having 0-4 C1-4 alkyl substituents are heated and molded to give products having good resistance to radiochem. degradation Thus, 60:40 ethylene-propene rubber 100, 2,2,4-trimethyl-1,2-dihydroquinoline 0.5, dicumyl peroxide 3, S 0.1, calcined clay 100, and 5,6-dimethylacenaphthylene (I) 10 parts were rolled at 100° and pressed 20 min at 180° to give I-grafted rubber composition having tensile strength 0.65 and 0.69 kg/mm2 before and after γ-irradiation in air to 100 Mrad, resp., and elongation 670 and 580%, resp., compared with 0.65, 0.45, 680, and 140, resp., for a similar composition without I.
IC C08J003-00; C08F032-08; C08K005-01; C09K003-12
CC 38-7 (Elastomers, Including Natural Rubber)
IT **76149-90-1**
RL: USES (Uses)
(graft, with improved resistance to radiochem. degradation)
IT **76149-90-1**
RL: USES (Uses)
(graft, with improved resistance to radiochem. degradation)
RN 76149-90-1 HCAPLUS
CN Acenaphthylene, 5,6-dimethyl-, polymer with ethene and 1-propene (9CI) (CA INDEX NAME)

CM 1

CRN 41002-83-9
CMF C14 H12

KATHLEEN FULLER EIC 1700 REMSEN 4B28 571/272-2505



CM 2

CRN 115-07-1
CMF C3 H6

$H_3C-CH=CH_2$

CM 3

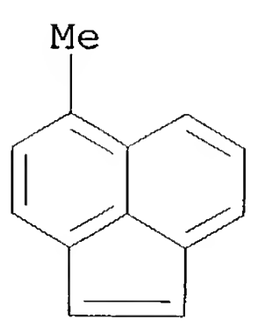
CRN 74-85-1
CMF C2 H4

$H_2C=CH_2$

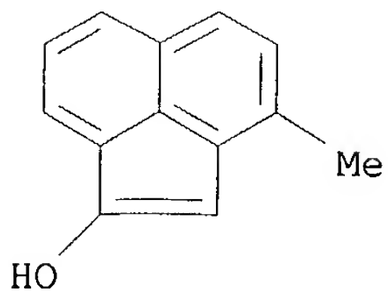
L53 ANSWER 28 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1976:508213 HCAPLUS
DN 85:108213
TI Electronic states of acenaphthylene. Linear dichroism in stretched polyethylene and magnetic circular dichroism
AU Thulstrup, Erik W.; Michl, Josef
CS Dep. Chem., Univ. Utah, Salt Lake City, UT, USA
SO Journal of the American Chemical Society (1976), 98(15), 4533-40
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English

AB Low-temperature absorption, linear dichroic, and magnetic circular dichroic spectroscopy of acenaphthylene (I) and its 1,2-dibromo (II), 3-, 4-, and 5-fluoro, and 5-Me derivs. confirm previous assignments of five electronic states, detect a new one, and determine the directions of magnetic dipole transition moments between excited states; energies, intensities, polarizations, and signs of B terms agree with results of π-electron calcns. Systematic introduction of doubly excited configurations has little effect on the results for excited states assigned to the first five observed transitions; it suggests, however, that the newly observed excited state is predominantly doubly excited. The energy of the lowest triplet state of I was measured by the O perturbation technique. Measurement of polarized absorption in stretched polyethylene ("stretched-sheet method") yields the correct absolute polarizations even for a nearly circular mol. such as I; the expected reversal of preferred orientation on going to II is observed The results demand a 2-parameter description of the orientation distribution and provide a good example for the inadequacy of 1-parameter

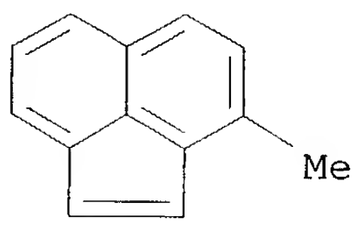
evaluation methods which are still occasionally used.
CC 22-8 (Physical Organic Chemistry)
IT 208-96-8 13019-33-5 17521-01-6 **19345-91-6** 20371-47-5
21502-72-7
RL: PRP (Properties)
(electron configuration of, spectra in relation to)
IT **19345-91-6**
RL: PRP (Properties)
(electron configuration of, spectra in relation to)
RN 19345-91-6 HCAPLUS
CN Acenaphthylene, 5-methyl- (8CI, 9CI) (CA INDEX NAME)



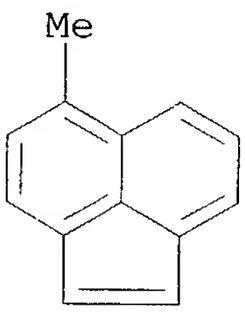
L53 ANSWER 29 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1976:104649 HCAPLUS
DN 84:104649
TI π,π-Biradicaloid hydrocarbons. The pleiadene family. II. A doubly excited state of pleiadene
AU Kolc, Jaroslav; Downing, John W.; Manzara, Anthony P.; Michl, Josef
CS Dep. Chem., Univ. Utah, Salt Lake City, UT, USA
SO Journal of the American Chemical Society (1976), 98(4), 930-7
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
AB Eleven excited singlet states in the uv spectra of pleiadene, five methylpleiadenes, and two dimethylpleiadenes were assigned for the absorptions between 200 and 1000 nm. Ti-electron calcns. (PPP-CI) account for the results and indicate that the second lowest excited state is doubly excited. The second transition involves promotion of both electrons from the highest occupied MO to the lowest unoccupied MO.
CC 22-2 (Physical Organic Chemistry)
IT **59012-07-6**
RL: PRP (Properties)
(3-methylacenaphthylene from)
IT **19345-94-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with benzyne)
IT **19345-91-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with benzyne)
IT **59012-07-6**
RL: PRP (Properties)
(3-methylacenaphthylene from)
RN 59012-07-6 HCAPLUS
CN 1-Acenaphthylenol, 3-methyl- (9CI) (CA INDEX NAME)



IT **19345-94-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with benzyne)
RN 19345-94-9 HCAPLUS
CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)

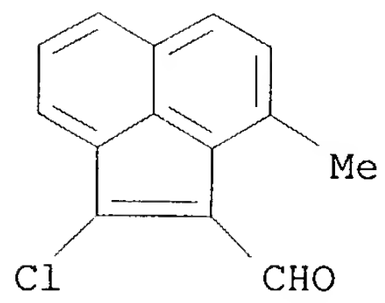


IT **19345-91-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with benzyne)
RN 19345-91-6 HCAPLUS
CN Acenaphthylene, 5-methyl- (8CI, 9CI) (CA INDEX NAME)

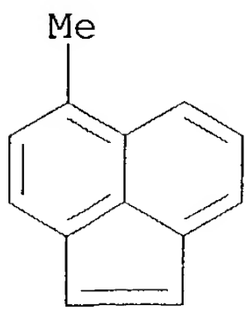


L53 ANSWER 30 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1976:74018 HCAPLUS
DN 84:74018
TI Application of the method for thiophene heterocycle synthesis using sodium sulfide to the preparation of sulfur analogs of polycyclic aromatic hydrocarbons
AU Cagniant, Paul; Kirsch, Gilbert
CS Fac. Sci., Univ. Metz, Metz, Fr.
SO Comptes Rendus des Seances de l'Academie des Sciences, Serie C: Sciences Chimiques (1975), 281(11), 393-5
CODEN: CHDCAQ; ISSN: 0567-6541
DT Journal
LA French
OS CASREACT 84:74018
AB Naphtho[1,2-b]thiophene, thieno[3,2-g]benzothiophene, acenaphtho[1,2-b]thiophene, acenaphtho[4,5-b]thiophene, phenanthro[1,2-b]thiophene, phenanthro[4,3-b]thiophene, and acephenanthro[7,8-b]thiophene ring systems

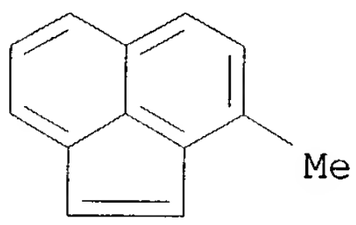
were prepared by Vilsmeyer-Haack formylation of tetrahydroarom. ketones, condensation of the chloroformyl derivs. with Na2S-BrCHCRCO2Et (R = H, Me), and aromatization with dichlorodicyanoquinone.
CC 27-9 (Heterocyclic Compounds (One Hetero Atom))
IT 3262-03-1P 49665-04-5P 58231-27-9P 58231-28-0P 58231-29-1P
58231-30-4P 58231-31-5P 58231-32-6P 58231-33-7P
58231-34-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with sodium sulfide and bromoalkanoate)
IT **58231-30-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with sodium sulfide and bromoalkanoate)
RN 58231-30-4 HCAPLUS
CN 1-Acenaphthylenecarboxaldehyde, 2-chloro-8-methyl- (9CI) (CA INDEX NAME)



L53 ANSWER 31 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1973:546892 HCAPLUS
DN 79:146892
TI Cationic polymerization of acenaphthylene and methylacenaphthylenes
AU Cohen, S.; Belliard, P.; Marechal, E.
CS Inst. Natl. Super. Chim. Ind. Rouen, Mont-Saint-Aignan, Fr.
SO Polymer (1973), 14(8), 352-4
CODEN: POLMAG; ISSN: 0032-3861
DT Journal
LA English
AB The kinetics and reactivity ratio compared with PhCH:CH2 were determined for the polymerization of acenaphthylenet(I) [208-96-8] initiated by stannic chloride [7646-78-8]. Comparison of exptl. with Hueckel MO and Pople complete neglect of differential overlap MO calcns. of stabilization energies indicated the contribution of ring strain to the reactivity of I. Reactivity ratios and stabilization energies were determined for the polymerization of 1-methylacenaphthylene [19345-99-4], 3-methylacenaphthylene [**19345-94-9**], and 5-methylacenaphthylene [**19345-91-6**].
CC 35-4 (Synthetic High Polymers)
IT **19345-91-6 19345-94-9** 19345-99-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(polymerization of, reactivity in)
IT **19345-91-6 19345-94-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(polymerization of, reactivity in)
RN 19345-91-6 HCAPLUS
CN Acenaphthylene, 5-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 19345-94-9 HCAPLUS
CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)



L53 ANSWER 32 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1973:72715 HCAPLUS
DN 78:72715
TI Cationic polymerization and copolymerization of methylacenaphthylenes
AU Belliard, Patrick; Marechal, Ernest
CS Lab. Chim. Macromol., Inst. Natl. Super. Chim. Ind., Rouen, Fr.
SO Bulletin de la Societe Chimique de France (1972), (11), 4255-75
CODEN: BSCFAS; ISSN: 0037-8968
DT Journal
LA French
AB High purity 1-methylacenaphthylene (I) [19345-99-4], 3-methylacenaphthylene [**19345-94-9**], and 5-methylacenaphthylene [**19345-91-6**] were prepared; steric hindrance in I prevented polymerization and copolymn., and only the lower oligomers were formed. Data for poly(3-methylacenaphthylene) [**38723-82-9**], poly(5-methylacenaphthylene) [**38723-83-0**], 3-methylacenaphthylene-styrene copolymer [**38720-69-3**], and 5-methylacenaphthylene-styrene copolymer [**38720-70-6**] agreed with CNDO II (J. A. Pople, 1965) calcns. rather than with Hueckel calcns. The effects of 5-C ring strain on acenaphthylene carbocation formation were discussed.
CC 35-4 (Synthetic High Polymers)
Section cross-reference(s): 26
IT **19345-97-2** **41002-77-1** **41002-78-2**
41002-79-3 **41002-80-6** **41002-81-7**
41002-82-8 **41002-83-9** **41002-84-0**
41002-85-1 **41002-86-2** **41002-87-3**
41002-88-4 **41002-89-5** **41002-90-8**
41002-91-9 **41002-92-0** **41002-93-1**
41002-94-2 **41002-95-3** **41002-96-4**
41002-97-5 **41002-98-6** **41002-99-7**
41003-00-3 **41003-01-4** **41003-02-5**
41003-03-6 **41003-04-7** **41003-05-8**
41082-61-5 **41082-62-6** 41237-23-4
RL: PRP (Properties)
(mol. orbitals of, calcn. of)
IT 85-08-5P 2435-82-7P **19345-91-6P** **19345-94-9P**
19345-99-4P **38723-82-9P** **38723-83-0P** 40908-02-9P
40908-03-0P 40908-04-1P 41002-74-8P

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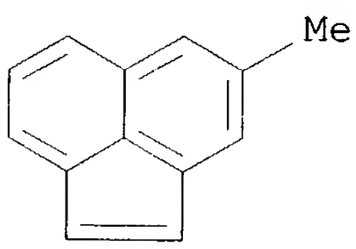
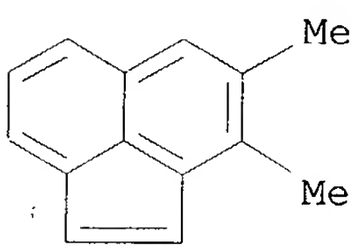
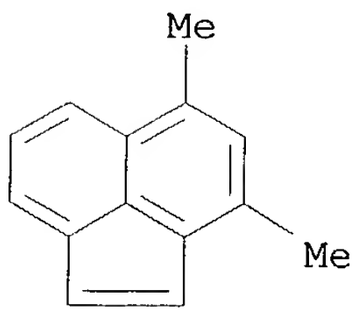
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 30347-44-5P **38720-69-3P 38720-70-6P** 40908-05-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, reactivity ratios in)
IT **19345-97-2 41002-77-1 41002-78-2**
41002-79-3 41002-80-6 41002-81-7
41002-82-8 41002-83-9 41002-84-0
41002-85-1 41002-86-2 41002-87-3
41002-88-4 41002-89-5 41002-90-8
41002-91-9 41002-92-0 41002-93-1
41002-94-2 41002-95-3 41002-96-4
41002-97-5 41002-98-6 41002-99-7
41003-00-3 41003-01-4 41003-02-5
41003-03-6 41003-04-7 41003-05-8
41082-61-5 41082-62-6
RL: PRP (Properties)
(mol. orbitals of, calcn. of)
RN 19345-97-2 HCAPLUS
CN Acenaphthylene, 4-methyl- (8CI, 9CI) (CA INDEX NAME)



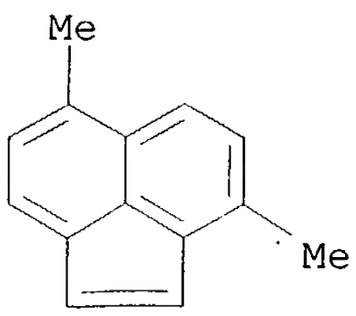
RN 41002-77-1 HCAPLUS
CN Acenaphthylene, 3,4-dimethyl- (9CI) (CA INDEX NAME)



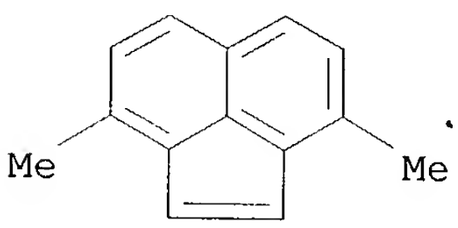
RN 41002-78-2 HCAPLUS
CN Acenaphthylene, 3,5-dimethyl- (9CI) (CA INDEX NAME)



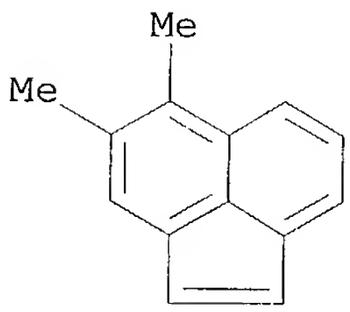
RN 41002-79-3 HCAPLUS
CN Acenaphthylene, 3,6-dimethyl- (9CI) (CA INDEX NAME)



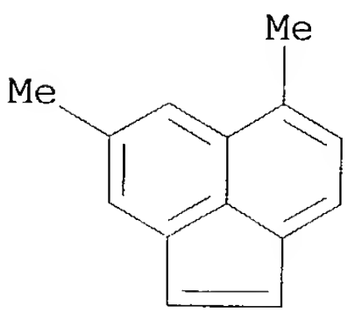
RN 41002-80-6 HCAPLUS
CN Acenaphthylene, 3,8-dimethyl- (6CI, 9CI) (CA INDEX NAME)



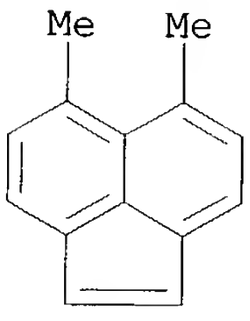
RN 41002-81-7 HCAPLUS
CN Acenaphthylene, 4,5-dimethyl- (9CI) (CA INDEX NAME)



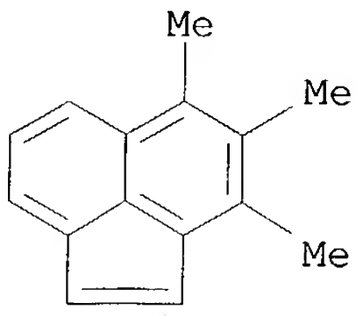
RN 41002-82-8 HCAPLUS
CN Acenaphthylene, 4,6-dimethyl- (9CI) (CA INDEX NAME)



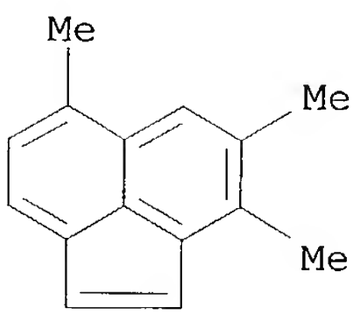
RN 41002-83-9 HCAPLUS
CN Acenaphthylene, 5,6-dimethyl- (6CI, 9CI) (CA INDEX NAME)



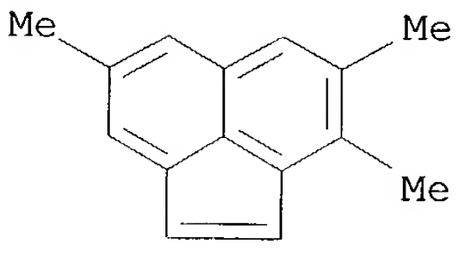
RN 41002-84-0 HCAPLUS
CN Acenaphthylene, 3,4,5-trimethyl- (9CI) (CA INDEX NAME)



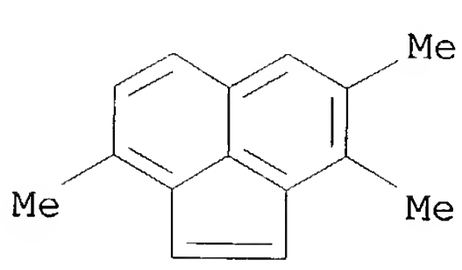
RN 41002-85-1 HCAPLUS
CN Acenaphthylene, 3,4,6-trimethyl- (9CI) (CA INDEX NAME)



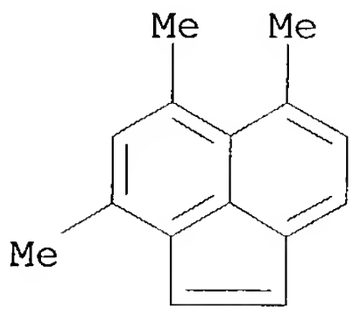
RN 41002-86-2 HCAPLUS
CN Acenaphthylene, 3,4,7-trimethyl- (9CI) (CA INDEX NAME)



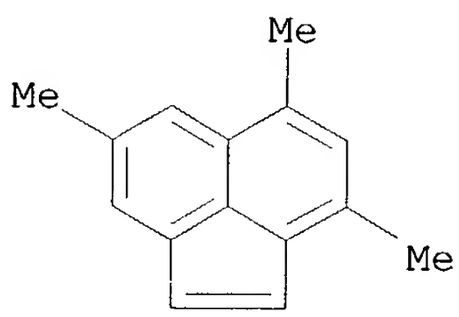
RN 41002-87-3 HCAPLUS
CN Acenaphthylene, 3,4,8-trimethyl- (9CI) (CA INDEX NAME)



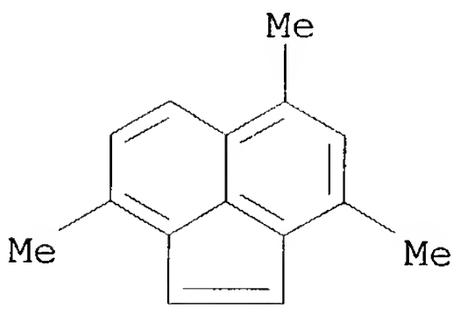
RN 41002-88-4 HCAPLUS
CN Acenaphthylene, 3,5,6-trimethyl- (9CI) (CA INDEX NAME)



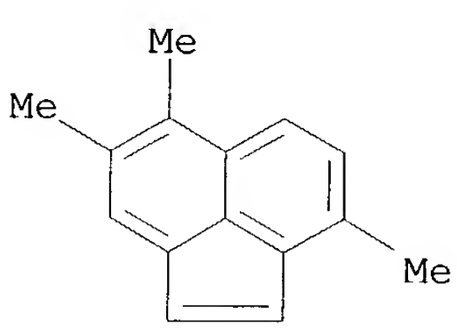
RN 41002-89-5 HCAPLUS
CN Acenaphthylene, 3,5,7-trimethyl- (9CI) (CA INDEX NAME)



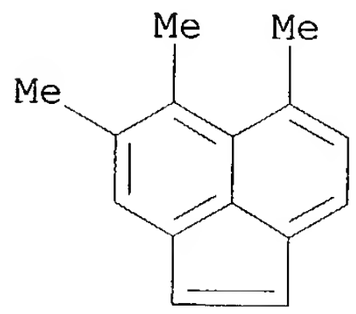
RN 41002-90-8 HCAPLUS
CN Acenaphthylene, 3,5,8-trimethyl- (9CI) (CA INDEX NAME)



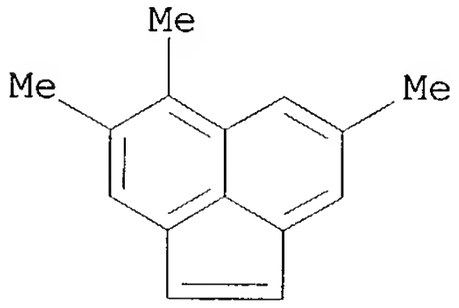
RN 41002-91-9 HCAPLUS
CN Acenaphthylene, 3,6,7-trimethyl- (9CI) (CA INDEX NAME)



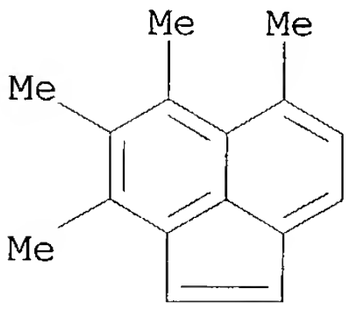
RN 41002-92-0 HCAPLUS
CN Acenaphthylene, 4,5,6-trimethyl- (9CI) (CA INDEX NAME)



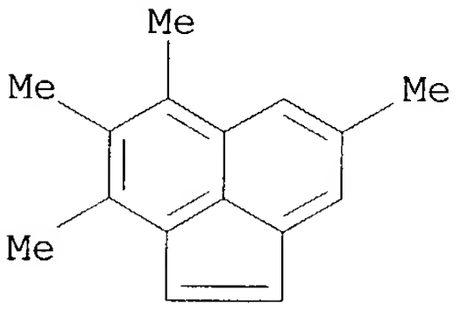
RN 41002-93-1 HCAPLUS
CN Acenaphthylene, 4,5,7-trimethyl- (9CI) (CA INDEX NAME)



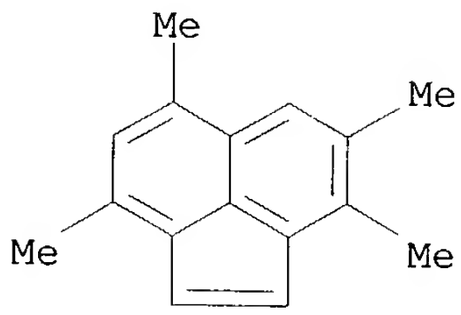
RN 41002-94-2 HCAPLUS
CN Acenaphthylene, 3,4,5,6-tetramethyl- (9CI) (CA INDEX NAME)



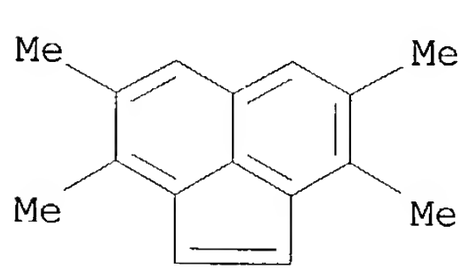
RN 41002-95-3 HCAPLUS
CN Acenaphthylene, 3,4,5,7-tetramethyl- (9CI) (CA INDEX NAME)



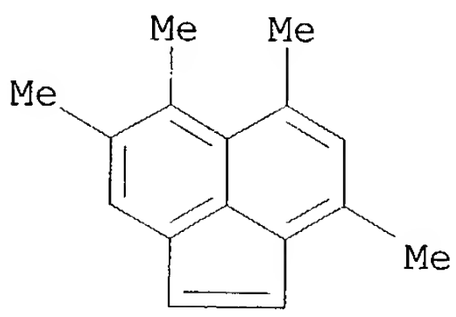
RN 41002-96-4 HCAPLUS
CN Acenaphthylene, 3,4,6,8-tetramethyl- (9CI) (CA INDEX NAME)



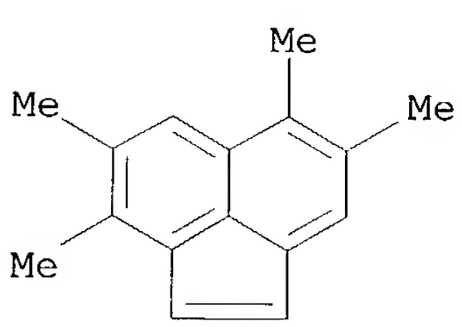
RN 41002-97-5 HCAPLUS
CN Acenaphthylene, 3,4,7,8-tetramethyl- (9CI) (CA INDEX NAME)



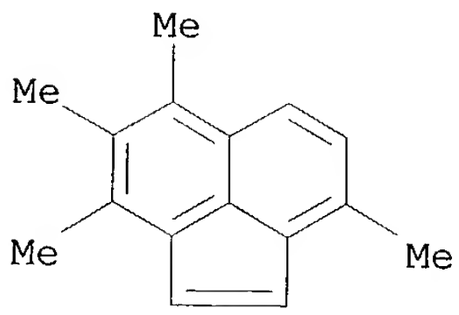
RN 41002-98-6 HCAPLUS
CN Acenaphthylene, 3,5,6,7-tetramethyl- (9CI) (CA INDEX NAME)



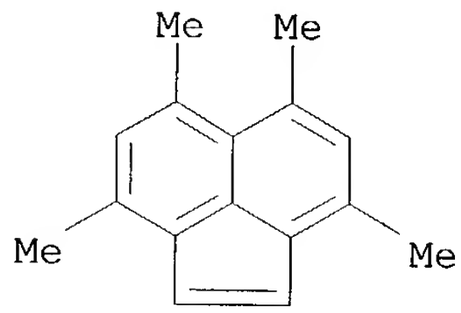
RN 41002-99-7 HCAPLUS
CN Acenaphthylene, 3,4,6,7-tetramethyl- (9CI) (CA INDEX NAME)



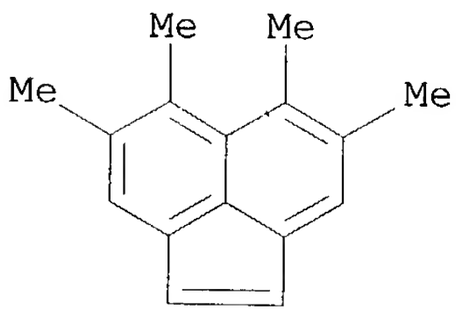
RN 41003-00-3 HCAPLUS
CN Acenaphthylene, 3,4,5,8-tetramethyl- (9CI) (CA INDEX NAME)



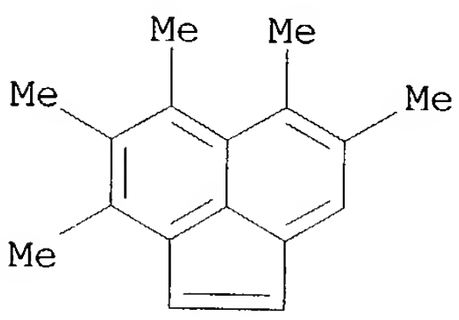
RN 41003-01-4 HCAPLUS
CN Acenaphthylene, 3,5,6,8-tetramethyl- (9CI) (CA INDEX NAME)



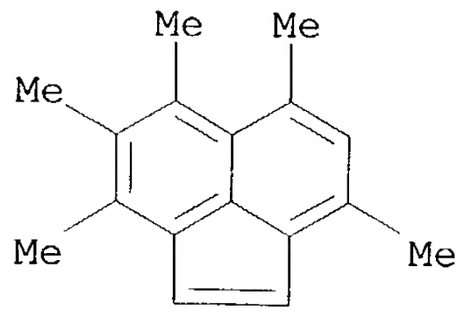
RN 41003-02-5 HCAPLUS
CN Acenaphthylene, 4,5,6,7-tetramethyl- (9CI) (CA INDEX NAME)



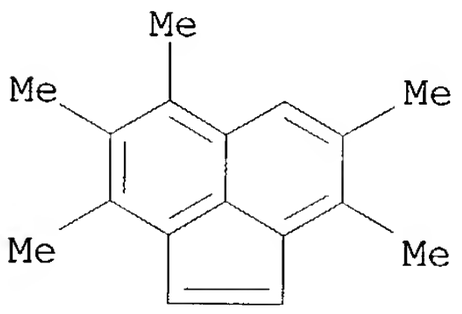
RN 41003-03-6 HCAPLUS
CN Acenaphthylene, 3,4,5,6,7-pentamethyl- (9CI) (CA INDEX NAME)



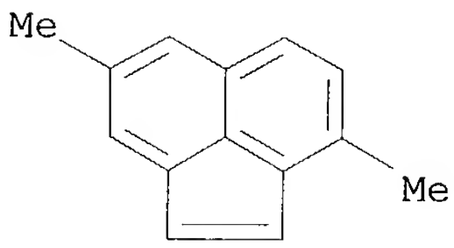
RN 41003-04-7 HCAPLUS
CN Acenaphthylene, 3,4,5,6,8-pentamethyl- (9CI) (CA INDEX NAME)



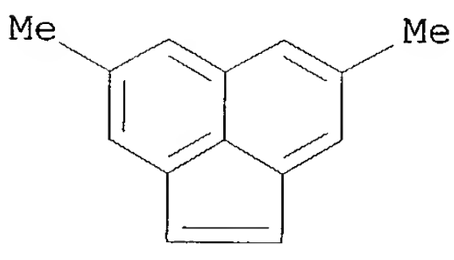
RN 41003-05-8 HCAPLUS
CN Acenaphthylene, 3,4,5,7,8-pentamethyl- (9CI) (CA INDEX NAME)



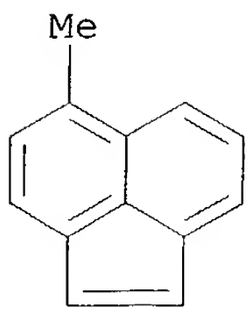
RN 41082-61-5 HCAPLUS
CN Acenaphthylene, 3,7-dimethyl- (9CI) (CA INDEX NAME)



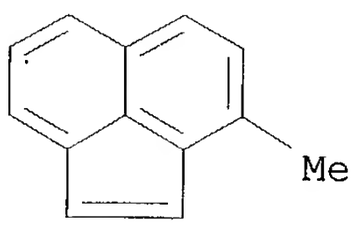
RN 41082-62-6 HCAPLUS
CN Acenaphthylene, 4,7-dimethyl- (9CI) (CA INDEX NAME)



IT **19345-91-6P 19345-94-9P 38723-82-9P**
38723-83-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 19345-91-6 HCAPLUS
CN Acenaphthylene, 5-methyl- (8CI, 9CI) (CA INDEX NAME)



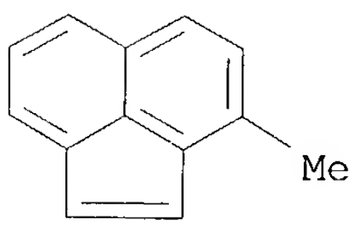
RN 19345-94-9 HCAPLUS
CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 38723-82-9 HCAPLUS
CN Acenaphthylene, 3-methyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

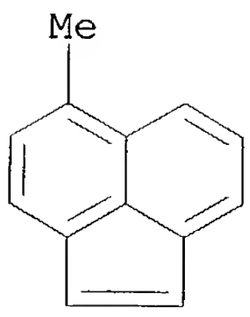
CRN 19345-94-9
CMF C13 H10



RN 38723-83-0 HCAPLUS
CN Acenaphthylene, 5-methyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 19345-91-6
CMF C13 H10



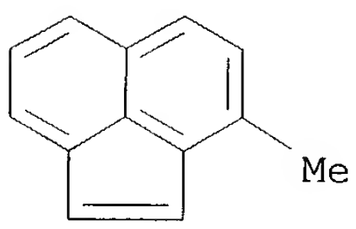
IT **38720-69-3P 38720-70-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, reactivity ratios in)
RN 38720-69-3 HCAPLUS

KATHLEEN FULLER EIC 1700 REMSEN 4B28 571/272-2505

CN Acenaphthylene, 3-methyl-, polymer with ethenylbenzene (9CI) (CA INDEX NAME)

CM 1

CRN 19345-94-9
CMF C13 H10



CM 2

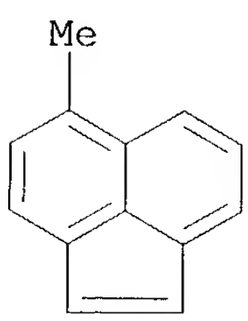
CRN 100-42-5
CMF C8 H8

H_2C═CH─Ph

RN 38720-70-6 HCAPLUS
CN Acenaphthylene, 5-methyl-, polymer with ethenylbenzene (9CI) (CA INDEX NAME)

CM 1

CRN 19345-91-6
CMF C13 H10



CM 2

CRN 100-42-5
CMF C8 H8

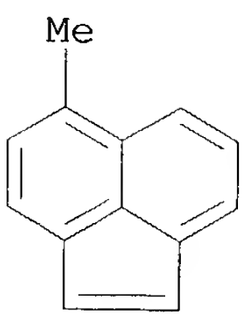
H_2C═CH─Ph

L53 ANSWER 33 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1973:72624 HCAPLUS
DN 78:72624

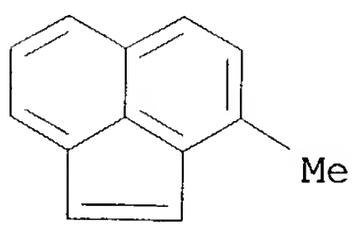
KATHLEEN FULLER EIC 1700 REMSEN 4B28 571/272-2505

TI Influence of the nature and position of substituents on the cationic polymerization of some aromatic monomers
AU Marechal, E.
CS Lab. Chim. Macromol., Inst. Natl. Super. Chim. Ind., Rouen, Fr.
SO Journal of Macromolecular Science, Chemistry (1973), 7(2), 433-60
CODEN: JMCHBD; ISSN: 0022-233X
DT Journal
LA English
AB Studies of the cationic polymerization of methylated and methoxylated monomers by

reactivity expts. and by quatum chemical theory indicated that although the results from the methods often agreed, discrepancies developed due to side phenomena. The phenomena included preliminary isomerization of the monomer, the ring strain effect, the effect of a substituent on monomer planarity, and complex formation.
CC 35-1 (Synthetic High Polymers)
IT 95-15-8 100-42-5, reactions 100-80-1 208-96-8 232-54-2 232-55-3
268-40-6 271-89-6 611-15-4 612-15-7 622-97-9 626-20-0 637-69-4
707-96-0 769-25-5 787-61-1 2039-89-6 2039-90-9 2234-20-0
3469-07-6 3469-08-7 3937-24-4 5379-20-4 6380-23-0 7530-35-0
13400-02-7 14568-68-4 16657-08-2 17055-36-6 17598-03-7
19345-91-6 19345-94-9 19345-97-2 19345-99-4
21897-50-7 22430-63-3 22484-28-2 23288-07-5 23288-08-6
23288-09-7 23288-10-0 23288-11-1 24345-63-9 24387-09-5
24407-19-0 27831-13-6 27973-23-5 28715-26-6 30566-10-0
34985-47-2 35074-19-2 35074-20-5 39240-15-8 40243-62-7
40243-64-9 40243-65-0 40243-66-1 40243-67-2 40243-68-3
40243-69-4 40243-70-7 40243-71-8 40243-72-9 40243-73-0
40243-74-1 40243-75-2 40243-78-5 40243-79-6 40243-84-3
40243-87-6 40243-89-8 40243-90-1 40243-91-2 40269-87-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(polymerization of, quantum chemical in relation to cationic)
IT **19345-91-6 19345-94-9 19345-97-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(polymerization of, quantum chemical in relation to cationic)
RN 19345-91-6 HCAPLUS
CN Acenaphthylene, 5-methyl- (8CI, 9CI) (CA INDEX NAME)

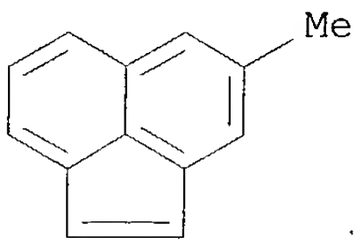


RN 19345-94-9 HCAPLUS
CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)



KATHLEEN FULLER EIC 1700 REMSEN 4B28 571/272-2505

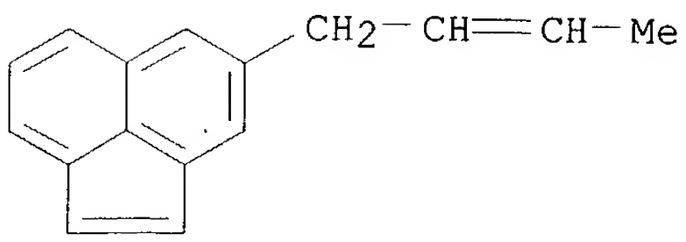
RN 19345-97-2 HCAPLUS
CN Acenaphthylene, 4-methyl- (8CI, 9CI) (CA INDEX NAME)



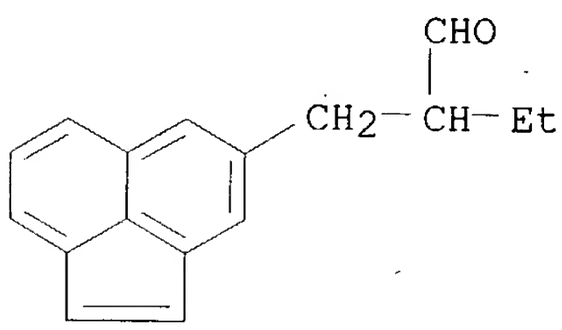
L53 ANSWER 34 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1972:405179 HCAPLUS
DN 77:5179
TI 3- and 4-Formylpentane mixtures
IN Himmele, Walter; Aquila, Werner
PA Badische Anilin- & Soda-Fabrik AG
SO Ger. Offen., 8 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2051319	A	19720427	DE 1970-2051319	19701020
PRAI	DE 1970-2051319		19701020		

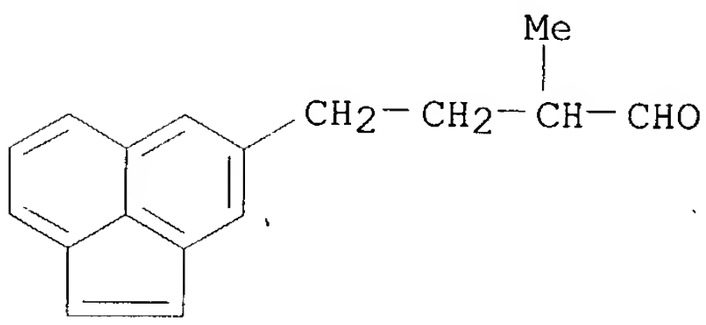
AB Five mixts. of RR1CHCH2CHEtCHO (I) and RR1CHCH2CH2CHMeCHO [II; R = Ph or o-MeC6H4; R1 = H, Me, Ph, or PhCH2, or RR1CH = 1,2,3,4-tetrahydro-1-naphthyl or acenaphthenyl], useful as perfumes, were prepared by hydroformylation of RR1CHCH2CH:CHMe (III) in the presence of dimeric cyclooctadienylrhodium chloride (IV) at 100°/700 atm gage and the aldehydes formed optionally hydrogenated and acetylated. Thus, III (R = o-MeC6H4, R1 = H) 176, C6H6300, and IV 0.05 part were heated 6 hr at 100°/700 atmospheric gage 1:1 CO-H pressure to give 177 parts mixture of I (R = o-MeC6H4, R1 = H) and II (R = o-MeC6H4, R1 = H) of flowery odor. The mixture (168 parts) was hydrogenated 12 hr over Raney Ni in MeOH at 80°/50 atmospheric to give 121 parts mixture of o-MeC6H4-(CH2)3CHMeCH2OH and o-MeC6H4CH2CH2CHEtCH2OH, which was refluxed 1 hr with Ac2O to give a mixture of the acetates.
IC C07C
CC 25-15 (Noncondensed Aromatic Compounds)
Section cross-reference(s): 26, 62
IT 6047-69-4 36613-03-3 **36613-06-6** 36666-03-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydroformylation of, catalysts for)
IT 33856-83-6P 36612-96-1P 36612-97-2P 36612-98-3P 36612-99-4P
36613-01-1P 36613-02-2P 36613-04-4P 36613-05-5P **36613-07-7P**
36613-08-8P 36613-11-3P 36613-13-5P 36613-14-6P
36613-15-7P 36613-16-8P 36613-17-9P 36613-18-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **36613-06-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydroformylation of, catalysts for)
RN 36613-06-6 HCAPLUS
CN Acenaphthylene, 4-(2-butenyl)- (9CI) (CA INDEX NAME)



IT **36613-07-7P 36613-08-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 36613-07-7 HCAPLUS
CN 4-Acenaphthylenepropanal, α-ethyl- (9CI) (CA INDEX NAME)



RN 36613-08-8 HCAPLUS
CN 4-Acenaphthylenebutanal, α-methyl- (9CI) (CA INDEX NAME)

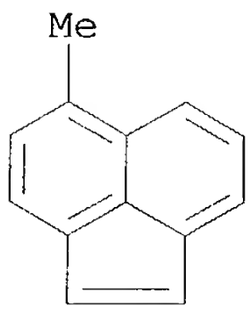


L53 ANSWER 35 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1968:458969 HCAPLUS
DN 69:58969
TI Constituents of cigaret smoke. XI. The isolation and synthesis of acenaphthylenes and macrocyclic polyolefins
AU Entwistle, I. D.; Johnstone, R. A. W.
CS Univ. Liverpool, Liverpool, UK
SO Journal of the Chemical Society [Section] C: Organic (1968), (14), 1818-22
CODEN: JSOOAX; ISSN: 0022-4952
DT Journal
LA English
GI For diagram(s), see printed CA Issue.
AB Acenaphthylene, the monomethylacenaphthylenes, such as I, and some dimethylacenaphthylenes were identified in cigarette smoke condensate. Some of the acenaphthylenes were synthesized, as was also a perhydromacrocycle cembrane (II). The possible formation of aromatic compounds from macrocyclic polyolefins is discussed, and the isolation of such a macrocycle from cigarette smoke is described. The mass spectra of some acenaphthylenes are described.
CC 26 (Condensed Aromatic Compounds)

IT 1786-12-5P 19335-98-9P 19345-88-1P 19345-89-2P 19345-90-5P
19345-91-6P 19345-92-7P 19345-93-8P
19345-94-9P 19345-95-0P 19345-96-1P
19345-97-2P 19345-98-3P 19345-99-4P
19346-00-0P 19346-01-1P 19346-02-2P
19346-03-3P 19346-04-4P 19346-05-5P 19346-06-6P
19346-07-7P 19346-08-8P 19346-09-9P 19346-10-2P 19565-21-0P
20526-63-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **19345-91-6P 19345-92-7P 19345-94-9P**
19345-95-0P 19345-97-2P 19345-98-3P
19346-00-0P 19346-01-1P 19346-02-2P
19346-03-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

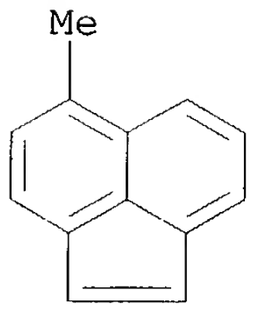
RN 19345-91-6 HCAPLUS
CN Acenaphthylene, 5-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 19345-92-7 HCAPLUS
CN Acenaphthylene, 5-methyl-, compd. with 1,3,5-trinitrobenzene (1:1) (8CI)
(CA INDEX NAME)

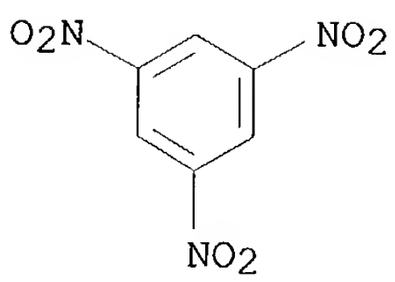
CM 1

CRN 19345-91-6
CMF C13 H10

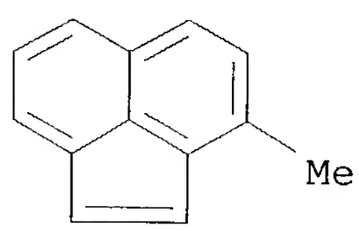


CM 2

CRN 99-35-4
CMF C6 H3 N3 O6



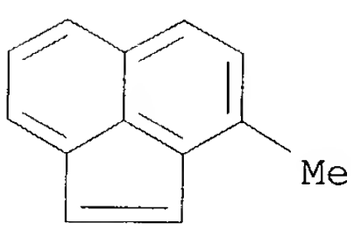
RN 19345-94-9 HCAPLUS
CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 19345-95-0 HCAPLUS
CN Acenaphthylene, 3-methyl-, compd. with 1,3,5-trinitrobenzene (1:1) (8CI)
(CA INDEX NAME)

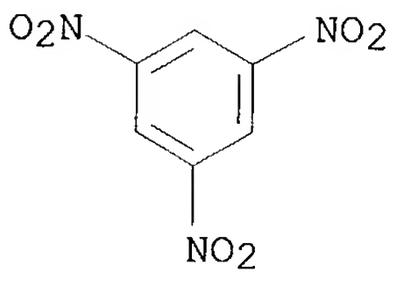
CM 1

CRN 19345-94-9
CMF C13 H10

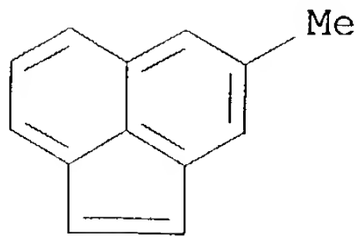


CM 2

CRN 99-35-4
CMF C6 H3 N3 O6



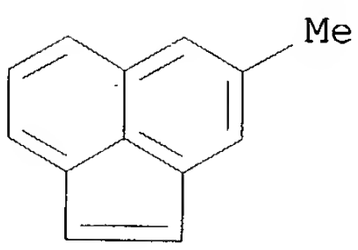
RN 19345-97-2 HCAPLUS
CN Acenaphthylene, 4-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 19345-98-3 HCAPLUS
CN Acenaphthylene, 4-methyl-, compd. with 1,3,5-trinitrobenzene (1:1) (8CI) (CA INDEX NAME)

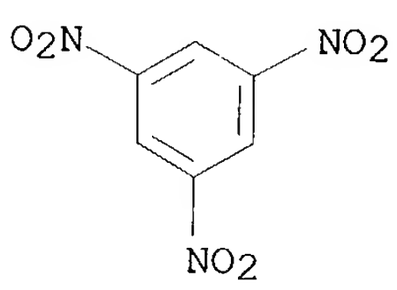
CM 1

CRN 19345-97-2
CMF C13 H10

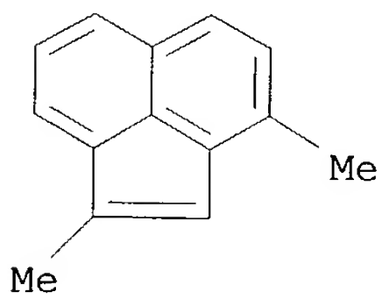


CM 2

CRN 99-35-4
CMF C6 H3 N3 O6



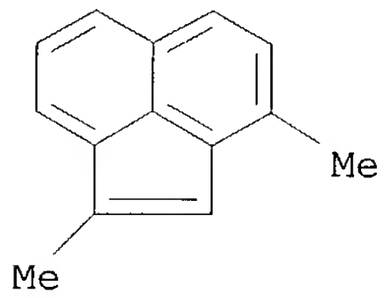
RN 19346-00-0 HCAPLUS
CN Acenaphthylene, 1,3-dimethyl- (8CI) (CA INDEX NAME)



RN 19346-01-1 HCAPLUS
CN Acenaphthylene, 1,3-dimethyl-, compd. with 1,3,5-trinitrobenzene (1:1) (8CI) (CA INDEX NAME)

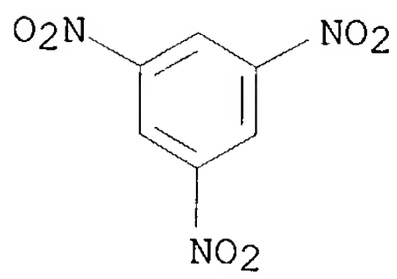
CM 1

CRN 19346-00-0
CMF C14 H12

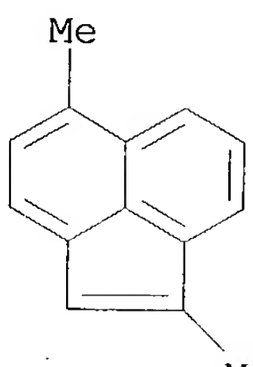


CM 2

CRN 99-35-4
CMF C6 H3 N3 O6



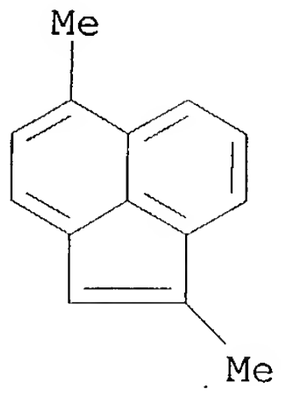
RN 19346-02-2 HCAPLUS
CN Acenaphthylene, 1,5-dimethyl- (8CI) (CA INDEX NAME)



RN 19346-03-3 HCAPLUS
CN Acenaphthylene, 1,5-dimethyl-, compd. with 1,3,5-trinitrobenzene (1:1) (8CI) (CA INDEX NAME)

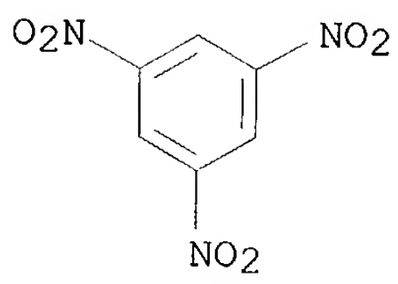
CM 1

CRN 19346-02-2
CMF C14 H12



CM 2

CRN 99-35-4
CMF C6 H3 N3 O6



L53 ANSWER 36 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1968:16234 HCAPLUS
DN 68:16234
TI Tables of quantum chemical data. XIV. Energy characteristics of some hydrocarbons with exocyclic methylene group
AU Tichy, Milos; Zahradnik, Rudolf
CS Ustav Hyg. Prace Chorob Povolani, Prague, Czech.
SO Collection of Czechoslovak Chemical Communications (1967), 32(12), 4485-91
CODEN: CCCCAK; ISSN: 0010-0765
DT Journal
LA English
AB Hueckel energy characteristics of derivs. formed by attaching a 2pz atomic orbital to an even alternant, odd alternant, or nonalternant hydrocarbon system were tabulated. Included are: nos. of π-electrons and of C-C σ-bonds, total π-electronic energy, sp. delocalization energy, energies of the 2 highest occupied and of the 2 lowest unoccupied M.O., and energy of the N → V1 transition.
CC 65 (General Physical Chemistry)
IT 497-20-1 539-79-7 4095-06-1 12341-14-9, Pentalene, 1,?-dihydro-1-methylene-, ion(1-) 12341-15-0, Pentalenylium, 2,?-dihydro-2-methylene- 12341-29-6, Azulenylium, 2,?-dihydro-2-methylene- 12341-30-9, Azulenylium, 1,?-dihydro-1-methylene- 12341-31-0, Azulene, 4,?-dihydro-4-methylene-, ion(1-) 12341-32-1, Azulenylium, 5,?-dihydro-5-methylene- 12341-33-2, Azulene, 6,?-dihydro-6-methylene-, ion(1-) 12341-56-9, Cyclohexadienylium, 6-methylene-3-phenyl- 12341-57-0, Heptalenylium, 1,?-dihydro-1-methylene- 12341-58-1, Heptalenylium, 2,?-dihydro-2-methylene- 12341-59-2, Heptalenylium, 3,?-dihydro-3-methylene- 12341-60-5, Acenaphthylenylium, 1,?-dihydro-1-methylene- **12341-61-6**, Acenaphthylene, 3,?-dihydro-3-methylene, ion(1-) 12341-62-7, Acenaphthylenylium, 4,?-dihydro-4-methylene- 12341-77-4, Anthracenylium,

1,?-dihydro-1-methylene- 12341-78-5, Anthracenylium,
2,?-dihydro-2-methylene- 12341-79-6, Anthracenylium,
9,?-dihydro-9-methylene- 12341-80-9, Phenanthrenylium,
4,?-dihydro-4-methylene- 12341-81-0, Phenanthrenylium,
3,?-dihydro-3-methylene- 12341-82-1, Phenanthrenylium,
2,?-dihydro-2-methylene- 12341-83-2, Phenanthrenylium,
1,?-dihydro-1-methylene- 12341-84-3, Phenanthrenylium,
9,?-dihydro-9-methylene- 12342-02-8, Fluoranthene, 3,?-dihydro-3-methylene-, ion(1-) 12342-03-9, Fluoranthene, 1,?-dihydro-1-methylene-, ion(1-) 12342-04-0, Fluoranthenylium, 2,?-dihydro-2-methylene- 12342-05-1, Fluoranthenylium, 7,?-dihydro-7-methylene- 12342-06-2, Fluoranthenylium, 8,?-dihydro-8-methylene- 12342-07-3, Acephenanthrylenylium, 2,?-dihydro-2-methylene- 12342-08-4, Acephenanthrylenylium, 10,?-dihydro-10-methylene- 12342-09-5, Acephenanthrylenylium, 8,?-dihydro-8-methylene- 12342-10-8, Acephenanthrylenylium, 5,?-dihydro-5-methylene- 12342-11-9, Acephenanthrylenylium, 4,?-dihydro-4-methylene- 12342-12-0, Aceanthrylenylium, 4,?-dihydro-4-methylene- 12342-13-1, Aceanthrylenylium, 8,?-dihydro-8-methylene- 12342-14-2, Pyrenylium, 2,?-dihydro-2-methylene- 12342-15-3, Aceanthrylenylium, 10,?-dihydro-10-methylene- 12342-16-4, Pyrenylium, 1,?-dihydro-1-methylene- 12342-17-5, Pyrenylium, 4,?-dihydro-4-methylene- 12342-18-6, Aceanthrylenylium, 2,?-dihydro-2-methylene- 12342-19-7, Aceanthrylenylium, 1,?-dihydro-1-methylene- 12342-29-9, Naphthacenylium, 5,?-dihydro-5-methylene- 12342-30-2, Naphthacenylium,
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2,?-dihydro-2-methylene- 12342-34-6, Benz[a]anthracenylium,
3,?-dihydro-3-methylene- 12342-35-7, Benz[a]anthracenylium,
4,?-dihydro-4-methylene- 12342-36-8, Benz[a]anthracenylium,
5,?-dihydro-5-methylene- 12342-37-9, Benz[a]anthracenylium,
6,?-dihydro-6-methylene- 12342-38-0, Benz[a]anthracenylium,
7,?-dihydro-7-methylene- 12342-39-1, Benz[a]anthracenylium,
8,?-dihydro-8-methylene- 12342-40-4, Benz[a]anthracenylium,
9,?-dihydro-9-methylene- 12342-41-5, Benz[a]anthracenylium,
10,?-dihydro-10-methylene- 12342-42-6, Benz[a]anthracenylium,
11,?-dihydro-11-methylene- 12342-43-7, Benz[a]anthracenylium,
12,?-dihydro-12-methylene- 12342-44-8, Triphenylenylium,
2,?-dihydro-2-methylene- 12342-45-9, Triphenylenylium,
1,?-dihydro-1-methylene- 12342-46-0, Chrysenylium, 5,?-dihydro-5-methylene- 12342-47-1, Chrysenylium, 6,?-dihydro-6-methylene- 12342-48-2, Chrysenylium, 1,?-dihydro-1-methylene- 12342-49-3, Chrysenylium, 2,?-dihydro-2-methylene- 12342-50-6, Chrysenylium, 3,?-dihydro-3-methylene- 12342-51-7, Chrysenylium, 4,?-dihydro-4-methylene- 12342-52-8, Benzo[c]phenanthrenylium, 1,?-dihydro-1-methylene- 12342-53-9, Benzo[c]phenanthrenylium, 2,?-dihydro-2-methylene- 12342-54-0, Benzo[c]phenanthrenylium, 3,?-dihydro-3-methylene- 12342-55-1, Benzo[c]phenanthrenylium, 4,?-dihydro-4-methylene- 12342-56-2, Benzo[c]phenanthrenylium, 5,?-dihydro-5-methylene- 12342-57-3, Benzo[c]phenanthrenylium, 6,?-dihydro-6-methylene- 12342-65-3, Benzo[k]fluoranthene, 3,?-dihydro-3-methylene-, ion(1-) 12342-74-4, Benz[a]aceanthrylenylium, 4,?-dihydro-4-methylene- 12342-75-5, Benz[a]aceanthrylenylium, 3,?-dihydro-3-methylene- 12342-76-6, Benz[a]aceanthrylenylium, 2,?-dihydro-2-methylene- 12342-77-7, Benz[a]aceanthrylenylium, 1,?-dihydro-1-methylene- 12342-78-8, Benz[a]aceanthrylenylium, 12,?-dihydro-12-methylene- 12342-79-9, Benz[a]aceanthrylenylium, 10,?-dihydro-10-methylene- 12342-80-2, Benz[a]aceanthrylenylium, 6,?-dihydro-6-methylene-

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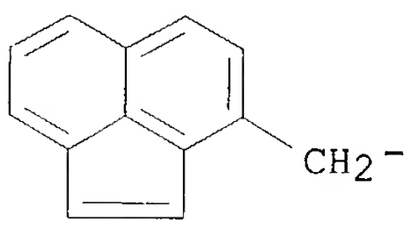
12342-81-3, Cyclopenta[fg]naphthacenylium, 1,?-dihydro-1-methylene-
12342-82-4, Cyclopenta[fg]naphthacenylium, 3,?-dihydro-3-methylene-
12342-83-5, Cyclopenta[fg]naphthacenylium, 5,?-dihydro-5-methylene-
13538-66-4 13538-67-5 19463-03-7 19463-04-8 19463-05-9
19463-06-0 19463-07-1 19463-08-2 19463-09-3 19463-10-6
19463-11-7 19463-12-8 19463-13-9 19463-14-0 19463-15-1
19463-16-2 19463-17-3 19463-18-4 19463-19-5 19463-20-8
19463-21-9 19463-22-0 19463-23-1 19463-24-2 19463-25-3
19463-26-4 19463-27-5 19463-28-6 19463-29-7 19463-30-0
19463-31-1 19463-32-2 19463-33-3 19463-34-4 19463-35-5
19463-36-6 19463-37-7 19463-38-8 20184-16-1
RL: PRP (Properties)
(energy levels of, calcn. of)

IT **12341-61-6**, Acenaphthylene, 3,?-dihydro-3-methylene, ion(1-)
RL: PRP (Properties)
(energy levels of, calcn. of)

RN 12341-61-6 HCAPLUS

CN Acenaphthylene, 3,?-dihydro-3-methylene-, ion(1-) (9CI) (CA INDEX NAME)



L53 ANSWER 37 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1966:35691 HCAPLUS
DN 64:35691
OREF 64:6588b-h,6589a-c
TI Pleiadene systems. II. Mechanism of acepleiadylene formation; a vinologous elimination in the acenaphthene series
AU Cava, M. P.; Merkel, K. E.; Schlessinger, R. H.
CS Ohio State Univ., Columbus
SO Tetrahedron (1965), 21(11), 3059-64
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
GI For diagram(s), see printed CA Issue.

AB cf. preceding abstract The conversion of 5,10-dihydroacepleiadene-5,10-diol (I) into acepleiadylene (II) by brief treatment with acid or by warming with p-MeC6H4SO2Cl in C5H5N appeared to involve 2 consecutive vinylogous eliminations. It was anticipated that the simpler model compound, 5-(α-hydroxybenzyl)acenaphthene (III) would similarly undergo vinylogous dehydration to the p-quinodimethane (IV), whose prototropic rearrangement would give the fully aromatic 5-benzylacenaphthylene (V). Acenaphthene (5.0 g.) and 3.7 ml. BzCl in 75 ml. C6H6 treated in 15 min. at 20° with 4.2 g. powdered AlCl3 and the mixture stirred 1 hr., poured into 100 ml. dilute HCl and extracted with Et2O, the isolated brown oil chromatographed on 100 g. neutral Al2O3 (Woelm, grade I) and eluted with C6H6 yielded 49% 5-benzoylacenaphthene (VI), m. 100-2°. VI (1.21 g.) and 0.5 g. NaBH4 in 70 ml. 4:3 C6H6-MeOH stirred 4 hrs. at 20° and the gelatinous residue on evaporation triturated with 10% aqueous NaOH yielded 95% III, m. 113-14° (C6H12). I (0.1 g.) and 0.1 g. p-MeC6H4SO2Cl in 20 ml. C5H5N refluxed (N atmospheric) 20 hrs. and the oily residue on evaporation

purified by chromatography over 20 g. neutral Al2O3 (Woelm, grade I), eluted with C6H12 and crystallized from C6H12 gave 58% V, m.5 8°, τ 5.54, 2.95 (CDCl3); N.M.R. spectrum of acenaphthylene, τ 2.92 (CDCl3). V (0.1 g.) in 50 ml. alc. hydrogenated over 0.12 g. 5% Pd-C 1 hr. and the filtered (Celite) solution evaporated in vacuo yielded 99% 5-benzylacenaphthene (VII), m. 111°. By use of a Soxhlet extractor, 0.4 g. VI was introduced into 300 ml. Et2O containing 0.65 g. LiAlH4 and 6.3 g. AlCl3 in 2 hrs., the mixture decomposed with 100 ml. H2O and extracted with 200 ml. Et2O to yield 93% VII, m. 111°, identical with the material obtained by reduction of VI. It was thus demonstrated that III could be converted to V by dehydration with p-MeC6H4SO2Cl in C5H5N. The analogous dehydration of 4-(α-hydroxybenzyl)acenaphthene (VIII) to 4-benzylacenaphthylene (IX) by way of a quinoid intermediate should not occur unless a hydride transfer mechanism involving carbonium ions were operative which would also be valid for conversion of III to V. An improved procedure for the synthesis of VIII was developed. Acenaphthene (100 g.) in 800 ml. AcOH stirred rapidly with addition of 125 ml. 70% aqueous HNO3 in 15 min. and the cooled mixture diluted to 2 l. with H2O yielded 87% 5-nitroacenaphthene, m. 104°. The nitro compound (50.0 g.), 2.5 g. 10% Pd-C, and 60 ml. 85% N2H4.H2O refluxed 45 min. in 1.0 l. 95% alc. and the hot filtered solution (Celite) diluted with H2O yielded 95% 5-aminoacenaphthene, m. 104°, acetylated with Ac2O-C5H5N to yield 95% 5-acetamidoacenaphthene, m. 190°. The amide (10.0 g.) in 900 ml. AcOH treated for 15 min. with 70 ml. 70% aqueous HNO3 and the mixture stirred 30 min., diluted with 2.0 l. H2O and the product refluxed 24 hrs. in 600 ml. alc. and 80 ml. 70% aqueous H2SO4, the hydrolysis mixture evaporated to .apprx.225 ml. and cooled to 10° gave 3.94 g, of dark red needles of 4-nitro-5-aminoacenaphthene (X), m. 235°. X (11.0 g.) in 150 ml. AcOH and 15 ml. concentrated H2SO4 added to 6.0 g. NaNO2 in 50 ml. concentrated H2SO4 at 0-20° and the mixture kept 1 hr. at 20°, the diazonium solution added slowly to a mixture of 14.0 g. CuSO4.5H2O, 180 ml. H3PO2, and 100 ml. 95% alc. and kept 1 hr. before dilution with 1.5 l. ice-H2O, extracted with 300 ml. EtOAc, and the isolated product chromatographed over 60 g. neutral Al2O3 (Woelm, grade II), eluted with C6H6, and crystallized from C6H6 gave 60% yield of 4-nitroacenaphthene, m. 130-2°. The nitro compound (20.0 g.) in 1.0 l. alc. containing 30 ml. 85% N2H4.H2O refluxed 2 hrs. with 2.0 g. 10% Pd-C and the filtered solution (Celite) evaporated to 100 ml., diluted with H2O to complete crystallization, and filtered gave 16.4 g. needles of 4-aminoacenaphthene, m. 88-9°. The amino compound (10.0 g.) in 25 ml. concentrated aqueous HCl and 115 ml. H2O diazotized at 0° with 4.5 g. NaNO2 in 50 ml. H2O, and the mixture stirred 1 hr., treated with 10.0 g. Hg(NO3)2 and 15.0 g. NaBr in 50 ml. H2O and the air-dried complex decomposed at 100° in 30 min. in the presence of 50.0 g. powdered NaBr, the decomposition residue extracted with C6H6, and the product purified from C6H6 by chromatography over 40 g. neutral Al2O3 gave a yellow solid, sublimed to yield 37% 4-bromoacenaphthene, m. 65-6°. The bromo compound (5.199 g.) and 3.6 g. CuCN refluxed 4 hrs. in 25 ml. freshly distilled N-methylpyrrolidone and the mixture poured into 15 ml. H2O and 4 ml. concentrated HCl containing 10.0 g. FeCl3, the mixture heated 20 min. on a steam bath and extracted with CHCl3, the isolated oily product chromatographed over 40 g. neutral Al2O3 (Woelm, grade I) and eluted with C6H6 yielded 71% 4-cyanoacenaphthene, m. 106-7°. The cyano derivative (0.105 g.) in 40 ml. Et2O stirred 4 hrs. at 20° with 3.0 ml. 3M ethereal PhMgBr and the mixture poured into 15 ml. concentrated aqueous HCl, filtered,

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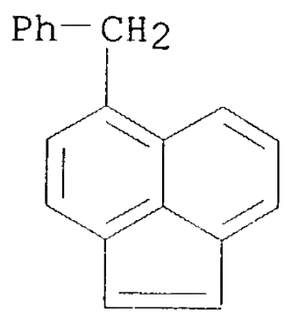
and the yellow imine HCl salt boiled in alc., the hydrolysis mixture diluted with 200 ml. CHCl3 and filtered from precipitated NH4Cl, the filtrate evaporated and
the residue crystallized from alc. gave an 82% yield of 4-benzoylacenaphthene, m. 97.0-8.5°. The ketone (1.0 g.) stirred 4 hrs. in 125 ml. Et2O with 1.0 g. LiAlH4 at 20° and the mixture diluted with 100 ml. H2O, the product isolated, and the white solid (0.88 g.) crystallized from C6H14 gave 88% yield of VIII, m. 86-7°. VIII (0.1 g.) and 0.15 g. p-MeC6H4SO2Cl in 20 ml. C5H5N refluxed (N atmospheric) 24 hrs. yielded only unchanged VIII.

CC 36 (Condensed Aromatic Compounds)
IT **4624-38-8**, Acenaphthylene, 5-benzyl-
(formation from α-phenyl-5-acenaphthenemethanol)
IT **4624-38-8**, Acenaphthylene, 5-benzyl-
(formation from α-phenyl-5-acenaphthenemethanol)
RN 4624-38-8 HCAPLUS
CN Acenaphthylene, 5-benzyl- (7CI, 8CI) (CA INDEX NAME)



L53 ANSWER 38 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1964:476383 HCAPLUS
DN 61:76383
OREF 61:13253g-h,13254a-d
TI Alkaline degradation of 1,1-disubstituted sulfonhydrazides. Synthesis of a pair of cyclic, benzylic hydrazines derived from acenaphthene and acenaphthylene
AU Carpino, Louis A.; Goewecke, Siegfried
CS Univ. of Massachusetts, Amherst
SO Journal of Organic Chemistry (1964), 29(10), 2824-30
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA Unavailable
GI For diagram(s), see printed CA Issue.
AB In order to test some hypotheses relating to the oxidation and sulfonhydrazide degradation of 1,1-disubstituted hydrazines, 2 appropriate model hydrazines have been prepared for further study, namely 2-amino-2,3-dihydro-1Hindeno[1,6,7-def]isoquinoline (I) and 2-amino-2,3,6,7-tetrahydro-1H-indeno[1,6,7-def]isoquinoline (II). Treatment of acenaphthene-5,6-dicarboxylic acid anhydride with N2H4.H2O gave the corresponding cyclic hydrazide (III), which was reduced by means of NaBH4 and LiBr to II. An alternate route to II involved LiAlH4 reduction of di-Me acenaphthene-5,6-dicarboxylate (IV) to the diol. Treatment of the diol with HBr gave the dibromide which upon treatment with tert-Bu carbazate and Et3N in HCONMe2 gave the carbo-tert-butoxy derivative (V) which was converted to II by cleavage with HCl. The most direct route to I involved treatment of 5,6-bis(bromomethyl)acenaphthene with N-bromosuccinimide to give the corresponding tribromide (VI). Treatment of VI with tert-Bu carbazate and Et3N in HCONMe2 was accompanied by dehydrobromination to give the protected, unsatd. hydrazine derivative (VII),

which on removal of the carbo-tert-butoxy group gave I. An alternate route to I involved bromination of IV with N-bromosuccinimide followed by dehydrobromination with LiBr in HCONMe2 to the unsatd. diester (VIII), reduction of which by means of LiAlH4 gave the unsatd. diol (IX). IX was converted to the dichloride by reaction with SOCl2 in C6H6 and the dichloride was cyclized to VII by reaction with tert-Bu carbazate and Et3N in HCONMe2. The ultraviolet and nuclear magnetic resonance spectra of the substituted acenaphthene and acenaphthylene derivs. obtained during the course of this work were examined and correlated with the spectra of the parent hydrocarbons.

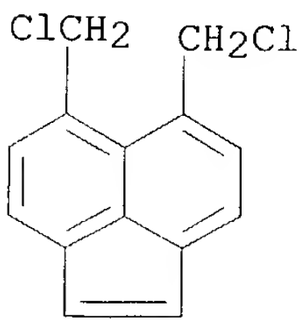
CC 36 (Condensed Aromatic Compounds)

IT 4599-95-5, Acenaphthene, 5,6-bis(bromomethyl)- 4599-96-6, 5,6-Acenaphthenedicarboxylic acid, dimethyl ester 4599-97-7, 5,6-Acenaphthenedimethanol 5699-00-3, 5,6-Acenaphthenedicarboxylic anhydride 5699-11-6, 5,6-Acenaphthenedicarboximide, N-amino- 33758-39-3, Carbaniloyl chloride, N-ethyl- 92152-70-0, Acenaphthene, 1-bromo-5,6-bis(bromomethyl)- **92152-76-6**, Acenaphthylene, 5,6-bis(chloromethyl)- **92254-00-7**, 5,6-Acenaphthylenedimethanol 92853-25-3, 5,6-Acenaphthenedicarboxylic acid, 1,2-dibromo-, dimethyl ester 92873-11-5, 5,6-Acenaphthenedicarboxylic acid, 1-bromo-, dimethyl ester 92964-95-9, 5,6-Acenaphthylenedicarboxylic acid, dimethyl ester 94873-12-8, 5,6-Acenaphthenedicarboximide, N-(benzylideneamino)- 95515-99-4, 1H-Indeno[6,7,1-def]isoquinoline, 2-amino-2,3,6,7-tetrahydro-, hydrochloride 98904-03-1, 2H-Indeno[6,7,1-def]isoquinoline-2-carbamic acid, 1,3,6,7-tetrahydro-, tert-butyl ester 100259-57-2, 1H-Indeno[6,7,1-def]isoquinoline, 2-(benzylideneamino)-2,3,6,7-tetrahydro- 106194-80-3, p-Toluenesulfonamide, N-(1,3,6,7-tetrahydro-2H-indeno[6,7,1-def]isoquinolin-2-yl)- 107101-72-4, 2H-Indeno[6,7,1-def]isoquinoline-2-carbamic acid, 1,3-dihydro-, tert-butyl ester
(preparation of)

IT **92152-76-6**, Acenaphthylene, 5,6-bis(chloromethyl)-
92254-00-7, 5,6-Acenaphthylenedimethanol
(preparation of)

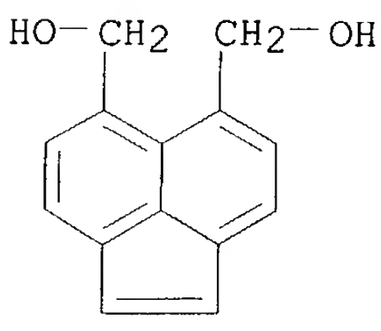
RN 92152-76-6 HCAPLUS

CN Acenaphthylene, 5,6-bis(chloromethyl)- (7CI) (CA INDEX NAME)



RN 92254-00-7 HCAPLUS

CN 5,6-Acenaphthylenedimethanol (7CI) (CA INDEX NAME)



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L53 ANSWER 39 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1961:124707 HCAPLUS
DN 55:124707
OREF 55:23456c-i,23457a-i,23458a-i,23459a-g
TI Polymerization of acenaphthylene induced by tritylsodium and halted by "at-complexes." IV
AU Wittig, Georg; Reppe, Hans G.; Eicher, Theophil
CS Univ. Tubingen, Germany
SO Ann. (1961), 643, 47-67
DT Journal
LA Unavailable
OS CASREACT 55:124707
GI For diagram(s), see printed CA Issue.
AB cf. CA 52, 1969g. (The term "at-complexes" signifies complexes formed by addition of an anion to a Lewis acid). Ph3CNa(I) polymerized acenaphthylene (II) by means of a carbanion chain. By the simultaneous presence of Ph3Al, the 1st step in the polymerization was halted after 1,2-addition of I to II by formation of III. In the presence of Ph3B, however, a 1,6-addition occurred, which formed IV. The acid hydrolysis of IV gave V, easily isomerized to 1-tritylacenaphthene (VI). The process leading to the formation of IV was explained by a π-complex formation between Ph3B and II. Thermal decomposition of trimethylammonium tetraphenylborate gave Ph3B, m. 151-2° (Me2CO-H2O). In 1 compartment of a double Schlenk tube was dissolved 9.5 millimoles Ph3B in 70 cc. absolute Et2O by warming under N, the solution filtered into the other compartment, treated with 9.5 millimoles I in 95 cc. Et2O, and cooled to -70° to give the at-complex I.BPh3. II m. 92-2.5° (70% EtOH). II (42 millimoles) in 20 cc. absolute Et2O added slowly from 1 compartment of a double Schlenk tube to 43 millimoles Ph3B in 360 cc. 0.09M Et2O-I contained in the other compartment, after 10 min. the precipitate (IV) filtered off under N, washed with Et2O under N, dissolved in 220 cc. distilled H2O, the solution acidified to pH 1 with 2N HCl, and extracted with 3:2 Et2O-C6H6 gave 1.5 g. V, m. 184-5° (decomposition) (CHCl3-EtOH). A sample of V dissolved in boiling AcOH and cooled gave VI, m. 241-2° (decomposition) [tetrahydrofuran (THF)-EtOH]. The mother liquors of V chromatographed on Al2O3 yielded addnl. V. Concentration of the Et2O solution decanted from IV gave 14% (Ph3C)2O2, m. 185-6° (dioxane); the Et2O filtrate washed with aqueous NaOH to remove Ph3B, evaporated, the residue chromatographed on Al2O3 in CCl4 and eluted with CCl4 gave 30% II, m. 91-2° (70% EtOH); further elution with CHCl3 gave 14% Ph3COH, m. 161-2° (cyclohexane). To 6 g. Ph3Al.Et2O in 10 cc. absolute Et2O was added 16 millimoles I in 150 cc. Et2O, the mixture treated with 16 millimoles II in 10 cc. absolute Et2O, shaken 45 hrs., heated 12 hrs. at 50°, the solution decomposed with 200 cc. 2N NaOH (all operations under N), and the precipitate filtered off to give 35% (including addnl. material from filtrate) crude VI, m. 230°. Li-Hg (from 100 g. Hg and 0.2 g. Li) was treated with 3.5 g. Ph3CCl (m. 113°) in 550 cc. absolute Et2O, the mixture shaken overnight, and the solution transferred to a stock burette to give Ph3CLi-Et2O; its content was determined by hydrolysis of an aliquot and titration with HCl. Ph3CLi (8 millimoles) in 500 cc. Et2O added to 8 millimoles 1-bromoacenaphthylene (m. 69-70°) in 20 cc. absolute Et2O, the solution concentrated to 50 cc., the precipitate filtered off, and washed with H2O gave 98% VI, m. 241-2° (THF-EtOH). A sample of VI (m. 241-2°) heated in vacuo while the bath temperature was gradually raised to 250° gave (at 0.2 mm.) II and (at 0.02 mm.) a small amount of VI and Ph3CH. To 3 millimoles VI in 140 cc. boiling AcOH was added dropwise

during 25 min. 60 millimoles CrO3 in 600 cc. AcOH, the solution boiled 1 hr., concentrated to 80 cc., and poured into 200 cc. H2O to give Ph3COH, m. 163-4° (MeOH with C); the aqueous filtrate treated with Na2SO3 and extracted 48 hrs. with 300 cc. Et2O gave 1,8-naphthalic acid anhydride, m. 271-2° (PhMe). NOCl (26 millimoles) in 25 cc. THF added dropwise during 5 min. to 12 millimoles VI in 250 cc. THF, after 30 min. the precipitate filtered off, and washed with 50 cc. THF gave 56% x-nitroso-y-chloro-1-trityldihydroacenaphthene (VII), m. 181-2° (decomposition) (CHCl3-EtOH). VII (1 g.) in 250 cc. AcOH boiled 20 min., the solution evaporated in vacuo, and the residue digested with 10 cc. MeOH gave 61% 2-acetoxy-1-tritylacenaphthene (VIII), m. 239-40° (THF-EtOH). Pb(OAc)4 (2 g.) in 50 cc. CHCl3 and 1 g. VI stirred 15 hrs., filtered, the filtrate concentrated, the residue washed with H2O, taken up in THF, the solution filtered, the filtrate concentrated, the residual tar dissolved in Et2O, and the solution concentrated to small volume gave 61% VIII, m. 240-40.5° (EtOH). VII (2 g.) in 2 l. AcOH boiled 15 hrs., the AcOH removed, the residue stirred with 20 cc. MeOH, and crystallized from AcOH gave 70% 1-tritylacenaphthylene (IX), m. 225-5.5°. IX was also obtained by boiling VIII in AcOH. 3,8-Dimethylacenaphthenone (m. 113-14°) (20 g.) in 1 l. absolute Et2O added slowly with stirring to 5 g. LiAlH4 in 200 cc. absolute Et2O, the mixture boiled 3 hrs., treated with 500 cc. 2N HCl, and the Et2O phase evaporated gave almost quant. 3,8-dimethyl-1-acenaphthenol (X), m. 114-15° (petr. ether). X (16 g.) in 160 cc. absolute pyridine treated during 10 min. at 0° with 8 g. AcCl in 20 cc. dry CHCl3 with stirring, kept 8 hrs. at 20°, poured into 1 l. H2O, extracted with Et2O, the extract washed with 4N HCl and aqueous NaHCO3, and fractionated gave 87% Ac derivative (XI) of X, b0.01 120-3°, m. 63-4° (MeOH). XI (10 g.) in 20 cc. quinoline and 180 cc. (HOCH2)2 (XII) boiled gently 30 min., cooled, poured into 500 cc. 4N HCl, extracted with Et2O, the Et2O phase washed with aqueous NaHCO3, and evaporated gave 80% 3,8-dimethylacenaphthylene (XIII), m. 56.5-7.5° (sublimation in vacuo, then 70% EtOH). XIII (5-millimoles) and 5 millimoles 1,3-diphenylisobenzofuran (XIV) in 15 cc. absolute xylene heated 15 hrs. at 130°, diluted with 100 cc. petr. ether, the precipitate manually freed from yellow needles (unchanged XIV), dissolved in 10 cc. hot xylene, the solution filtered, and the filtrate diluted with 100 cc. EtOH gave 29% adduct, m. 195.5-6.0°; from the mother liquor was isolated 48% XIII and 58% XIV. To 110 millimoles Ph3B suspended in 200 cc. absolute Et2O was added 11 millimoles XIII followed during 30 min. by 11 millimoles I in 100 cc. Et2O, after 12 hrs. the supernatant liquor decanted from a precipitate, the precipitate taken up in 100 cc. H2O, the solution acidified with 2N HCl, the resulting precipitate dissolved in C6H6, the solution washed with aqueous NaOH (to remove Ph3B), and concentrated to 15 cc. to give 850 mg. Ph3CH, m. 92-3° (EtOH) (the mother liquor contained 300 mg. material, chiefly tar); the decanted Et2O solution washed with aqueous NaOH, evaporated, the residue chromatographed on Al2O3, and eluted with C6H6 gave 1.60 g. Ph3CH, m. 88-92° (from the mother liquor was isolated 20 mg. p-benzhydryltetraphenylmethane (XV) and 14% XIII, m. 55-6.5°). An experiment with 2:1:1 Ph3B-XIII-I gave 91% Ph3CH, 22% XIII, and 38% tar. Freshly distilled EtO2CCOCl (0.31 mole) added at 0° to 0.31 mole AlCl3 in 150 cc. PhNO2 with stirring, the mixture treated dropwise during 1 hr. with 0.15 mole 1,8-C10H6Me2 (m. 64-5°) at 0-5°, kept 12 hrs. at 15°, and decomposed with 1 l. 1:1 concentrated HCl-ice H2O with stirring gave 69% Et 4,5-dimethyl-1-naphthylglyoxylate (XVI), b0.01 160-3°, m. 51-2° (MeOH). XVI (75 g.) refluxed with 93 g. KOH and 116 g.

80% $N_2H_4.H_2O$ in 580 cc. XII, diluted with 3 l. H_2O, filtered, and the filtrate acidified with concentrated HCl to pH 1 gave 86% 4,5-dimethyl-1-naphthaleneacetic acid (XVII), m. 184-5° (dilute EtOH with C). To 40 g. XVII in 500 cc. boiling $CHCl_3$ was added during 20 min. 51 g. freshly distilled $SOCl_2$ in an equal volume $CHCl_3$ with stirring, the mixture concentrated, the residual acid chloride taken up in 400 cc. $PhNO_2$, the solution added dropwise during 2 hrs. to 45 g. $AlCl_3$ in 300 cc. $PhNO_2$ (preheated to 70°) with stirring, stirred 36 hrs. at 20°, decomposed with 800 g. ice and 250 cc. concentrated HCl, the $PhNO_2$ phase steam distilled, the residue rubbed with MeOH, and sublimed at 160-5° (bath temperature)/0.01 mm. to give 70% 5,6-dimethylacenaphthenone (XVIII), m. 164-5° (EtOH with C). XVIII (25 g.) added to 10 g. $LiAlH_4$ in 1.2 l. absolute Et_2O with stirring, the mixture boiled 24 hrs., decomposed with 700 cc. 2N HCl, the precipitate present at the interphase filtered off, and combined with a slight amount product present in the Et_2O gave 80% 5,6-dimethyl-1-acenaphthenol (XIX), m. 192-3° (EtOH). To 20 g. XIX in 100 cc. absolute pyridine was added dropwise at 0° 16 g. AcCl in 20 cc. $CHCl_3$ with stirring, the mixture stirred 12 hrs. at 0°, decomposed with 600 cc. H_2O, and the product isolated with Et_2O to give 90% Ac derivative (XX) of XIX, m. 84-5° (EtOH). XX (10 g.) in 20 cc. quinoline and 180 cc. XII boiled gently 30 min., decomposed with HCl, the crude product isolated with Et_2O (as described for XIII), pulverized, extracted with petr. ether, the extract concentrated to 100 cc., chromatographed on Al_2O_3, and eluted with petr. ether gave 64% 5,6-dimethylacenaphthylene (XXI), m. 98-9° (petr. ether with C). XXI (5.26 millimoles) in 20 cc. EtOAc added to a prereduced suspension of 0.2 g. Pd-C in 15 cc. EtOAc and 5 cc. MeOH (after shaking 1 hr. 5.23 millimoles H absorbed) gave 5,6 dimethylacenaphthene, m. 167-9° (EtOH). XXI (5 millimoles) and 5 millimoles XIV in 15 cc. xylene heated 15 hrs. at 130° under N and diluted with 100 cc. petr. ether gave 84% adduct, m. 213.5-14.5° (iso-AmOH); from the mother liquor was isolated 10% XXI. To 23 millimoles Ph_3B suspended in 20 millimoles I in 170 cc. Et_2O was added gradually 20 millimoles XXI, the mixture shaken vigorously (the Ph_3B dissolved), after 1 hr. shaken and cooled to 0°, kept 12 hrs., the supernatant liquor decanted from the precipitate, the precipitate washed with absolute Et_2O, dissolved in 2 l. H_2O, the solution acidified, extracted with Et_2O, the extract washed with aqueous NaOH, and concentrated to 20 cc. to give 2.1 g. crude 1-trityl-5,6-dimethylacenaphthene (XXII); a sample dissolved in a little $CHCl_3$, the solution diluted with EtOH, and cooled to -50° gave XXII, m. 238-40° ($CHCl_3$-EtOH); the remaining crude XXII dissolved in boiling AcOH and the solution boiled 5 min. gave XXII, m. 256-8°, which was recrystd. 3 times from 95% BuOH to give XXII, m. 259-60° (decomposition), mixed m.p. (with material m. 238-40°) 238-43°; the infrared spectra of both prepns. were practically identical. PBr_3 (7 g.) in 10 cc. absolute Et_2O added dropwise with stirring to 3 g. XIX in 150 cc. absolute Et_2O at 0°, kept 1.5 hrs. at 0°, diluted with sufficient absolute Et_2O to effect solution, the solution washed rapidly with dilute aqueous $NaHCO_3$, dried, added with stirring to 0.1N I-Et_2O until a permanent red color formed, and treated with H_2O gave XXII, m.p. and mixed m.p. 259-60° (95% BuOH). 5,6-Dichloroacenaphthene (XXIII) (m. 167-8°) (58 g.) in 1 l. AcOH (distilled over $KMnO_4$) treated portionwise at 65° with 210 g. Pb_3O_4, heated 1 hr. at 80-90°, the solution poured into 2 l. ice H_2O, the supernatant solution decanted from a gummy precipitate, the precipitate dissolved in 400 cc. hot EtOH, the

solution treated with C, and cooled gave 1-acetoxy derivative (XXIV) of XXIII, m. 104-5° (EtOH). XXIV (50 g.) boiled 1.5 hrs. with 30 g. KOH in 500 cc. MeOH and diluted with 500 cc. H2O gave 80% 5,6-dichloro-1-acenaphthenol (XXV), m. 157-8° (C6H6 with C). XXV (30 g.) in 500 cc. C6H6 and a minute amount 4-MeC6H4SO3H heated 30 min. under a H2O separator (2 cc. H2O was formed), the solution washed with aqueous NaOH, concentrated, the residue taken up in petr. ether, the filtered solution chromatographed on Al2O3, and eluted with petr. ether gave 49% 5,6-dichloroacenaphthylene (XXVI), m. 161-1.5°. To 46 millimoles Ph3B and 20 millimoles XXVI in 150 cc. absolute Et2O was added portionwise 20 millimoles I in 200 cc. Et2O with stirring and the complex worked up as above to give 21% 1-trityl derivative of XXVI, m. 240-1° (decomposition) (BuOH); the Et2O solution yielded 8% XXVI, 39% Ph3CH, 3% XV, and 5% tar. The following compds. were prepared for spectral comparison studies. Finely powdered Ph3P.MeBr (65 millimoles) added to 60 millimoles BuLi in 100 cc. Et2O in an N atmospheric, the mixture shaken 0.5 hr., the solution of Ph3P:CH2 (XXVII) treated dropwise with 50 millimoles OC.CMe2.CH:CH.C6H4 (XXVIII) (b15 130.5-2.0°, n24D 1.5705) in 30 cc. absolute Et2O (exothermic reaction), shaken 40 hrs. at room temperature, decanted from precipitated Ph3PO, the Et2O phase and washings combined, treated with N NaOH, concentrated to 30 cc., filtered from more Ph3PO, and the filtrate worked up gave 5.2 g. H2C:C.CMe2.CH:CH.C6H4 (XXIX), b0.3 55.5-7.0°, n25D 1.5757, and Ph3PO (the total yield of Ph3PO was 8.6 g.). XXIX (10.4 millimoles in 40 cc. EtOAc hydrogenated with 0.3 g. Pd-C (20.7 millimoles H absorbed in 4 hrs.) gave 85% MeCH.CMe2.CH2.CH2.C6H4 (XXX), b16 113-14°. OC.CMe2.CH2.CH2.C6H4 (XXXI) (b15 131-2°, n20D 1.5424 (29 millimoles) in 50 cc. absolute Et2O treated as above with 36 millimoles XXVII in 80 cc. Et2O gave 4.2 g. H2C:C.CMe2.CH2.CH2.C6H4 (XXXII), b15 118.5-20.0°, n20D 1.5570. XXXII (2.3 g.) in 60 cc. EtOAc hydrogenated with 0.3 g. Pd-C gave XXX, b16 114-15°, n19.5D 1.5274, identical with XXX prepared above. To Ph3P:CHMe (XXXIII) solution (prepared from 65 millimoles Ph3P.EtBr and 61 millimoles BuLi in 100 cc. Et2O) was added slowly 41 millimoles XXVIII in 50 cc. absolute Et2O, shaken 1 week at room temperature, and worked up as usual to give 8.1 g. Ph3PO and 5.1 g. MeCH:C.CMe2.CH:CH.C6H4 (XXXIV), b0.05 62.5-3.0°, n18D 1.5803. Hydrogenation of 10.4 millimoles XXXIV in 50 cc. EtOAc with 0.3 g. Pd-C (20.7 millimoles H absorbed in 4 hrs.) gave 83% EtCH.CMe2.CH2.CH2.C6H4 (XXXV), b0.3 56-7°, n20D 1.5248. XXXI (40 millimoles) treated with 46 millimoles XXXIII in 120 cc. Et2O and shaken 46 hrs. at 20° gave 6.5 g. MeCH:C.CMe2.CH2.CH2.C6H4 (XXXVI), b0.4 70-70.5°, n20D 1.5568. Hydrogenation of 25 millimoles XXXVI in 50 cc. EtOAc with 0.5 g. Pd-C gave XXXV, b0.3 56-7°, n20D 1.5256, identical with XXXV prepared above. OC.CH: CH.CMe2.C6H4 (XXXVII) (m. 69-70.5°) (50 millimoles) treated as above with 60 millimoles XXVII in 160 cc. Et2O and heated 70 hrs. at 60° gave 43% Ph3PO and 1.8 g. H2C:C.CH:CH.CMe2.C6H4, b0.1 54-4.5°, n22D 1.5807. XXXVII (50 millimoles) treated as above with 60 millimoles XXXIII in 160 cc. Et2O and heated 50 hrs. at 60° gave 70% Ph3PO and 4.7 g. MeCH:C.CH:CH.CMe2.C6H4 (XXXVIII), b0.03 69.5-70.0°, n22D 1.5821. Hydrogenation (10 hrs.) of 6.4 millimoles XXXVIII in 60 cc. EtOAc with 0.5 g. Pd-C gave 1.2 g. EtCH.CH2.CH2.CMe2.C6H4 (XXXIX), b14 125-6°, n20D 1.5215. EtMgBr solution (from 13 g. EtBr and 2.5 g. Mg in 40 cc. absolute Et2O) combined at 0° with 10 g. OC.CH2.CH2.CMe2.C6H4 (b0.3 79-81°) in 30 cc. absolute Et2O, boiled 90 min., and decomposed with aqueous NH4Cl gave 9.5 g. HOCEt.CH2.CH2.CMe2.C6H4 (XL), b14 98-8.5°, m. 60-1°. XL

(9.5 g.) and a minute amount 4-MeC6H4SO3H boiled 12 hrs. under a H2O separator, washed with aqueous NaHCO3, and fractionated gave 88% EtC:CH.CH2.CMe2.C6H4 (XLI), b14 124.5-5.0°, n20D 1.5503. Hydrogenation (25 min.) of 16.6 millimoles XLI in 60 cc. EtOAc with 0.5 g. Pd-C gave 3 g. XXXIX, b14 125-6°, n20D 1.5217.

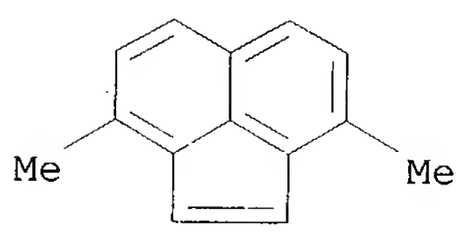
CC 10F (Organic Chemistry: Condensed Carbocyclic Compounds)

IT 7267-09-6, Acenaphthylene, 5,6-dichloro- **41002-80-6**, Acenaphthylene, 3,8-dimethyl- **41002-83-9**, Acenaphthylene, 5,6-dimethyl-
(preparation and reactions of)

IT **41002-80-6**, Acenaphthylene, 3,8-dimethyl- **41002-83-9**, Acenaphthylene, 5,6-dimethyl-
(preparation and reactions of)

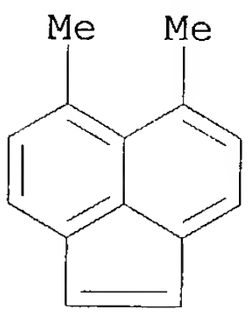
RN 41002-80-6 HCAPLUS

CN Acenaphthylene, 3,8-dimethyl- (6CI, 9CI) (CA INDEX NAME)



RN 41002-83-9 HCAPLUS

CN Acenaphthylene, 5,6-dimethyl- (6CI, 9CI) (CA INDEX NAME)



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